



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2024 – 07:49 AM EST

PDB ID : 6DHF
Title : RT XFEL structure of the one-flash state of Photosystem II (1F, S2-rich) at 2.08 Angstrom resolution
Authors : Kern, J.; Chatterjee, R.; Young, I.D.; Fuller, F.D.; Lassalle, L.; Ibrahim, M.; Gul, S.; Fransson, T.; Brewster, A.S.; Alonso-Mori, R.; Hussein, R.; Zhang, M.; Douthit, L.; de Lichtenberg, C.; Cheah, M.H.; Shevela, D.; Wersig, J.; Seufert, I.; Sokaras, D.; Pastor, E.; Weninger, C.; Kroll, T.; Sierra, R.G.; Aller, P.; Butryn, A.; Orville, A.M.; Liang, M.; Batyuk, A.; Koglin, J.E.; Carbajo, S.; Boutet, S.; Moriarty, N.W.; Holton, J.M.; Dobbek, H.; Adams, P.D.; Bergmann, U.; Sauter, N.K.; Zouni, A.; Messinger, J.; Yano, J.; Yachandra, V.K.
Deposited on : 2018-05-20
Resolution : 2.08 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36

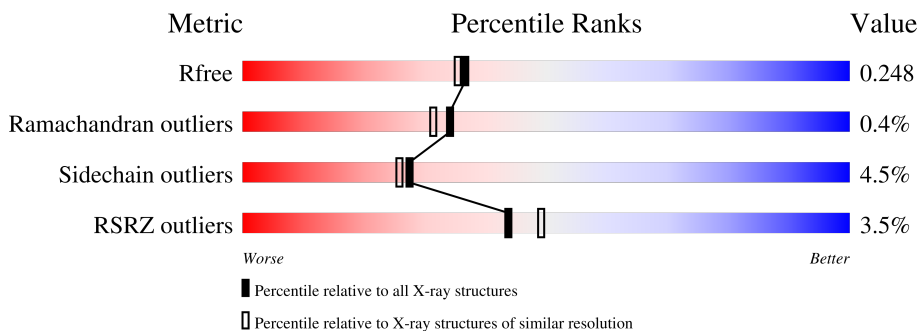
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

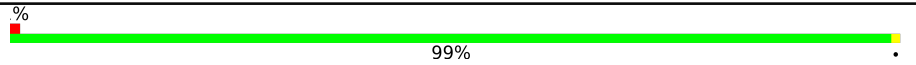
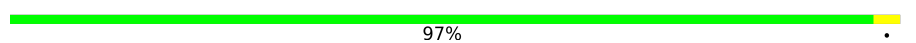
The reported resolution of this entry is 2.08 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6189 (2.10-2.06)
Ramachandran outliers	138981	6663 (2.10-2.06)
Sidechain outliers	138945	6664 (2.10-2.06)
RSRZ outliers	127900	6057 (2.10-2.06)

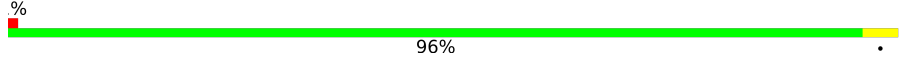
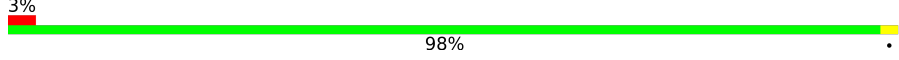
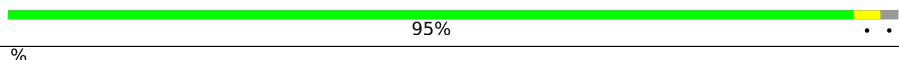
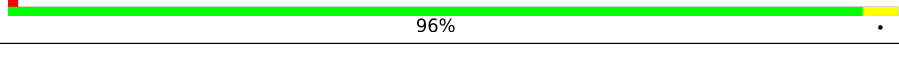
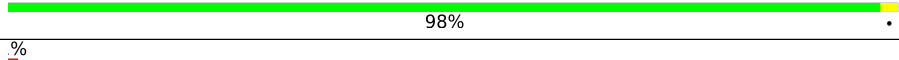
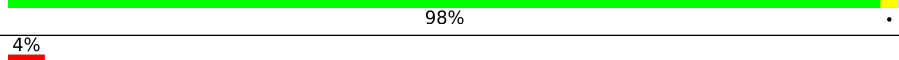
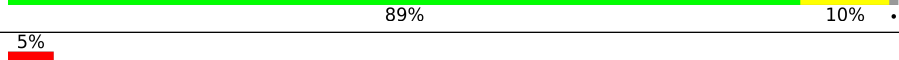
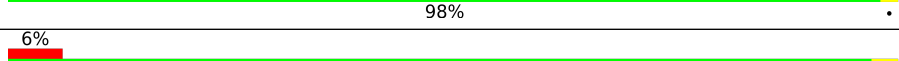
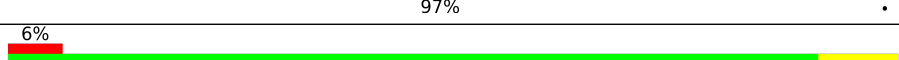
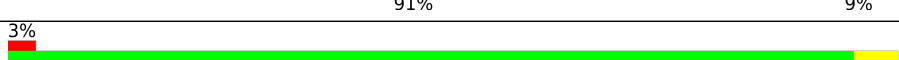
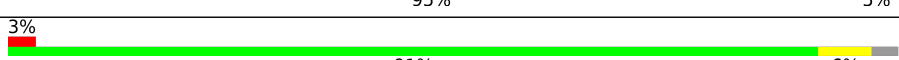
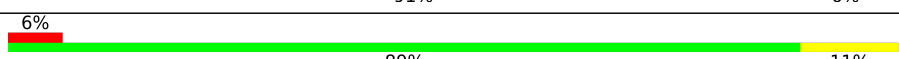
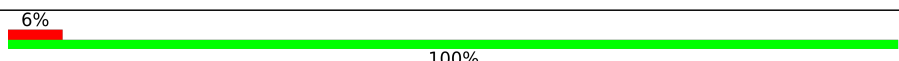
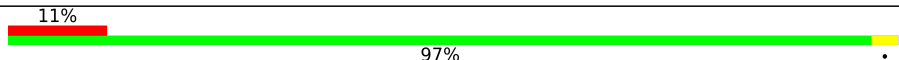
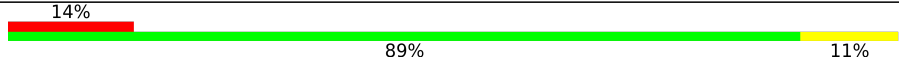
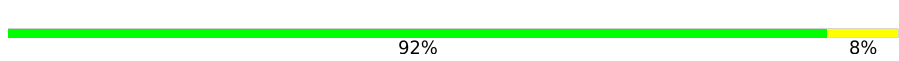

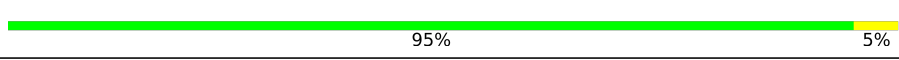
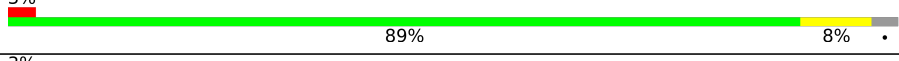
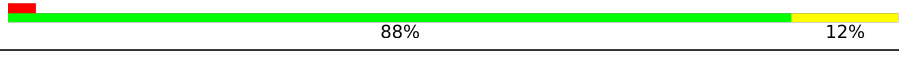
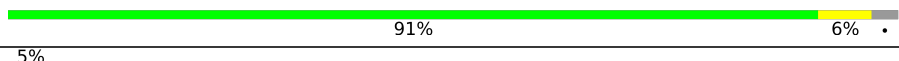
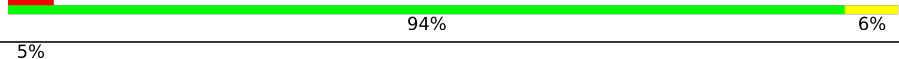
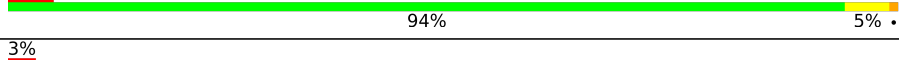


The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	334	 99%
1	a	334	 97%

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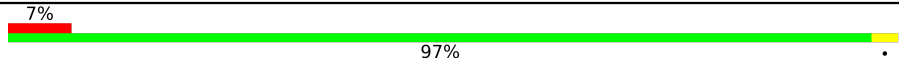
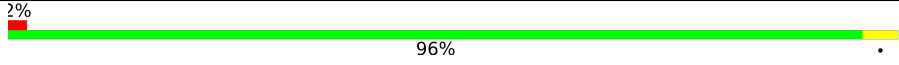
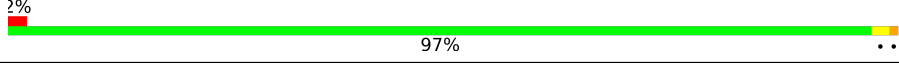
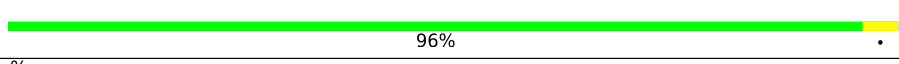
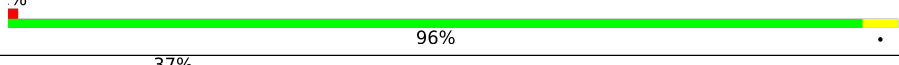
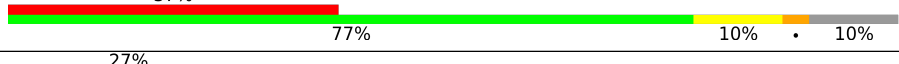
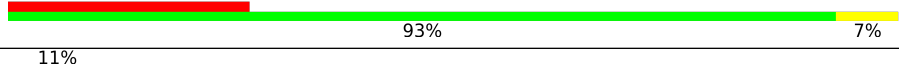
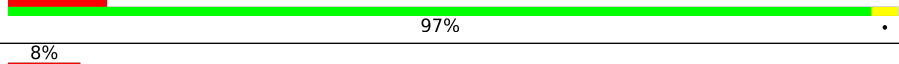
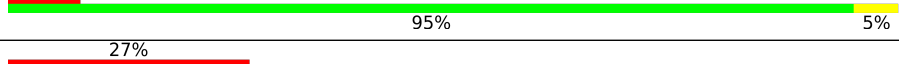
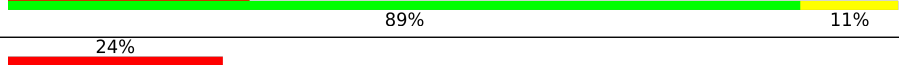



buster-report : 1.1.7 (2018)
 Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
 Refmac : 5.8.0158
 CCP4 : 7.0.044 (Gargrove)
 Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.36

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Mol	Chain	Length	Quality of chain
2	B	505	 96%
2	b	505	 98%
3	C	451	 95%
3	c	451	 96%
4	D	341	 98%
4	d	341	 98%
5	E	82	 89% 10%
5	e	82	 98%
6	F	34	 97%
6	f	34	 91% 9%
7	H	65	 95% 5%
7	h	65	 91% 6%
8	I	36	 89% 11%
8	i	36	 100%
9	J	36	 97%
9	j	36	 89% 11%
10	K	37	 92% 8%
10	k	37	 89% 11%
11	L	37	 95% 5%
11	l	37	 89% 8%
12	M	33	 88% 12%
12	m	33	 91% 6%
13	O	244	 94% 6%
13	o	244	 94% 5%
14	T	30	 87% 10%

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Mol	Chain	Length	Quality of chain
14	t	30	
15	U	97	
15	u	97	
16	V	137	
16	v	137	
17	Y	30	
17	y	30	
18	X	38	
18	x	38	
19	Z	62	
19	z	62	
20	R	34	
20	r	34	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	A	405	X	-	-	-
24	CLA	A	406	X	-	-	-
24	CLA	A	408	X	-	-	-
24	CLA	B	601	X	-	-	-
24	CLA	B	602	X	-	-	-
24	CLA	B	604	X	-	-	-
24	CLA	B	605	X	-	-	-
24	CLA	B	606	X	-	-	-
24	CLA	B	607	X	-	-	-
24	CLA	B	610	X	-	-	-
24	CLA	B	612	X	-	-	-
24	CLA	B	613	X	-	-	-
24	CLA	B	614	X	-	-	-
24	CLA	B	615	X	-	-	-
24	CLA	B	616	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	C	502	X	-	-	-
24	CLA	C	503	X	-	-	-
24	CLA	C	504	X	-	-	-
24	CLA	C	505	X	-	-	-
24	CLA	C	506	X	-	-	-
24	CLA	C	508	X	-	-	-
24	CLA	C	510	X	-	-	-
24	CLA	C	511	X	-	-	-
24	CLA	C	512	X	-	-	-
24	CLA	C	513	X	-	-	-
24	CLA	C	514	X	-	-	-
24	CLA	D	402	X	-	-	-
24	CLA	D	403	X	-	-	-
24	CLA	a	404	X	-	-	-
24	CLA	a	407	X	-	-	-
24	CLA	b	603	X	-	-	-
24	CLA	b	604	X	-	-	-
24	CLA	b	605	X	-	-	-
24	CLA	b	606	X	-	-	-
24	CLA	b	607	X	-	-	-
24	CLA	b	608	X	-	-	-
24	CLA	b	609	X	-	-	-
24	CLA	b	610	X	-	-	-
24	CLA	b	611	X	-	-	-
24	CLA	b	612	X	-	-	-
24	CLA	b	613	X	-	-	-
24	CLA	b	614	X	-	-	-
24	CLA	b	615	X	-	-	-
24	CLA	b	616	X	-	-	-
24	CLA	b	617	X	-	-	-
24	CLA	c	501	X	-	-	-
24	CLA	c	502	X	-	-	-
24	CLA	c	503	X	-	-	-
24	CLA	c	504	X	-	-	-
24	CLA	c	505	X	-	-	-
24	CLA	c	506	X	-	-	-
24	CLA	c	507	X	-	-	-
24	CLA	c	509	X	-	-	-
24	CLA	c	510	X	-	-	-
24	CLA	c	511	X	-	-	-
24	CLA	c	512	X	-	-	-
24	CLA	c	513	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	d	403	X	-	-	-
24	CLA	d	404	X	-	-	-
24	CLA	d	405	X	-	-	-
24	CLA	h	101	X	-	-	-

2 Entry composition [i](#)

There are 36 unique types of molecules in this entry. The entry contains 103698 atoms, of which 51491 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem II protein D1 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	334	5130	1717	2508	431	459	15	0	0	0
1	a	334	5118	1714	2499	431	459	15	0	0	0

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
2	B	505	7849	2631	3845	666	694	13	0	5	0
2	b	505	7789	2610	3811	665	690	13	0	0	0

- Molecule 3 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
3	C	442	6768	2249	3346	570	590	13	0	1	0
3	c	451	6911	2290	3411	587	610	13	0	2	0

- Molecule 4 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
4	D	341	5330	1800	2613	444	461	12	0	0	0
4	d	341	5342	1804	2619	444	463	12	0	1	0

- Molecule 5 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	81	Total	C	H	N	O	0	1	0
			1309	434	647	106	122			
5	e	82	Total	C	H	N	O	0	0	0
			1311	434	647	108	122			

- Molecule 6 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
6	F	34	Total	C	H	N	O	S	0	0	0
			556	187	281	45	42	1			
6	f	34	Total	C	H	N	O	S	0	0	0
			556	187	281	45	42	1			

- Molecule 7 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
7	H	65	Total	C	H	N	O	S	0	0	0
			1030	338	523	82	85	2			
7	h	63	Total	C	H	N	O	S	0	0	0
			1016	333	518	80	83	2			

- Molecule 8 is a protein called Photosystem II reaction center protein I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
8	I	36	Total	C	H	N	O	S	0	0	0
			607	200	311	46	49	1			
8	i	36	Total	C	H	N	O	S	0	0	0
			607	200	311	46	49	1			

- Molecule 9 is a protein called Photosystem II reaction center protein J.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
9	J	36	Total	C	H	N	O	S	0	0	0
			525	174	268	40	42	1			
9	j	36	Total	C	H	N	O	S	0	0	0
			516	172	261	40	42	1			

- Molecule 10 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	K	37	Total	C	H	N	O	0	1	0
			620	209	318	46	47			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	k	37	Total	C	H	N	O	0	0	0
			598	204	305	43	46			

- Molecule 11 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
11	L	37	Total	C	H	N	O	S	0	0	0
			620	202	316	48	53	1			
11	l	36	Total	C	H	N	O	0	0	0	
			600	197	304	47	52				

- Molecule 12 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
12	M	33	Total	C	H	N	O	S	0	0	0
			525	171	269	37	47	1			
12	m	32	Total	C	H	N	O	S	0	0	0
			518	168	267	36	46	1			

- Molecule 13 is a protein called Photosystem II manganese-stabilizing polypeptide.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
13	O	244	Total	C	H	N	O	S	0	1	0
			3730	1174	1850	317	385	4			
13	o	244	Total	C	H	N	O	S	0	0	0
			3718	1170	1844	317	383	4			

- Molecule 14 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
14	T	30	Total	C	H	N	O	S	0	0	0
			519	181	261	36	39	2			
14	t	30	Total	C	H	N	O	S	0	0	0
			512	180	256	36	38	2			

- Molecule 15 is a protein called Photosystem II 12 kDa extrinsic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	U	97	Total	C	H	N	O	0	0	0
			1546	491	772	129	154			
15	u	97	Total	C	H	N	O	0	0	0
			1546	491	772	129	154			

- Molecule 16 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
16	V	137	Total	C	H	N	O	S	0	0	0
			2134	675	1070	177	208	4			
16	v	137	Total	C	H	N	O	S	0	0	0
			2134	675	1070	177	208	4			

- Molecule 17 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
17	Y	27	Total	C	H	N	O	S	0	0	0
			404	128	208	35	30	3			
17	y	30	Total	C	H	N	O	S	0	0	0
			459	144	241	35	36	3			

- Molecule 18 is a protein called Photosystem II reaction center X protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
18	X	38	Total	C	H	N	O	0	0	0
			593	188	312	45	48			
18	x	38	Total	C	H	N	O	0	0	0
			593	188	312	45	48			

- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
19	Z	62	Total	C	H	N	O	S	0	0	0
			988	328	509	72	77	2			
19	z	62	Total	C	H	N	O	S	0	0	0
			986	326	509	72	77	2			

- Molecule 20 is a protein called Photosystem II protein Y.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
20	R	34	Total	C	H	N	O	0	0	0
			569	184	298	47	40			
20	r	31	Total	C	H	N	O	0	0	0
			461	154	234	40	33			

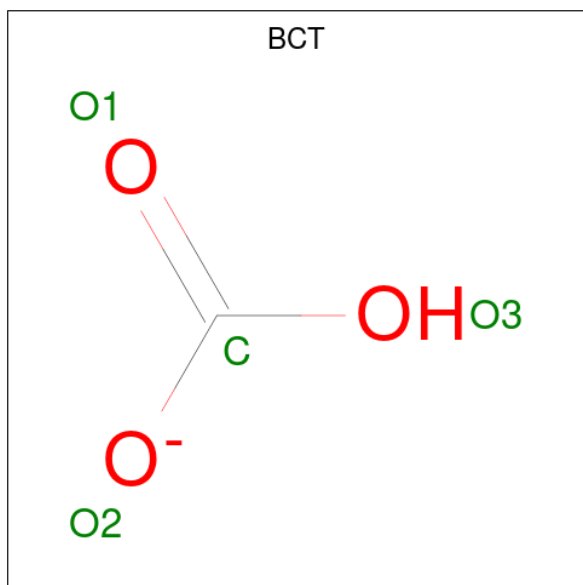
- Molecule 21 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	A	1	Total Fe 1 1	0	0
21	a	1	Total Fe 1 1	0	0

- Molecule 22 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

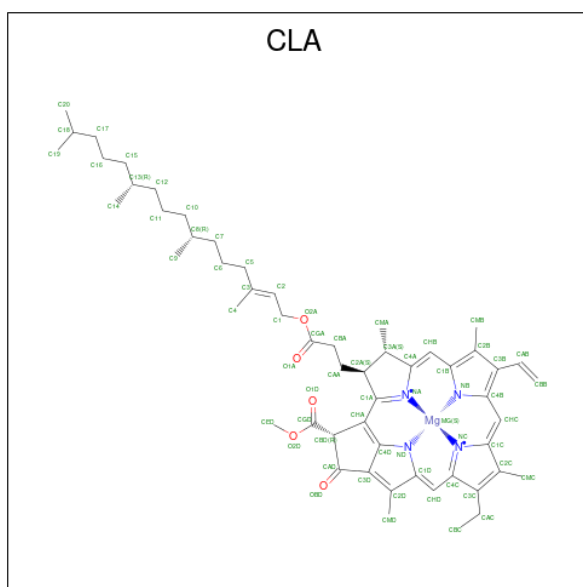
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	A	2	Total Cl 2 2	0	0
22	a	2	Total Cl 2 2	0	0

- Molecule 23 is BICARBONATE ION (three-letter code: BCT) (formula: CHO₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	A	1	Total C H O 5 1 1 3	0	0
23	d	1	Total C H O 5 1 1 3	0	0

- Molecule 24 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	Mg	N			O
24	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	A	1	Total	C	H	Mg	N	O	0	0
			102	44	48	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
24	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	C	1	Total	C	H	Mg	N	O	0	0
			117	49	58	1	4	5		
24	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	D	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	D	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	D	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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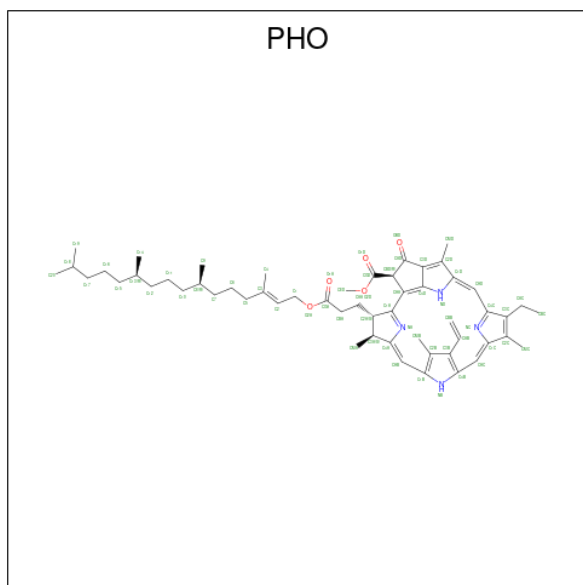
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
24	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	b	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
24	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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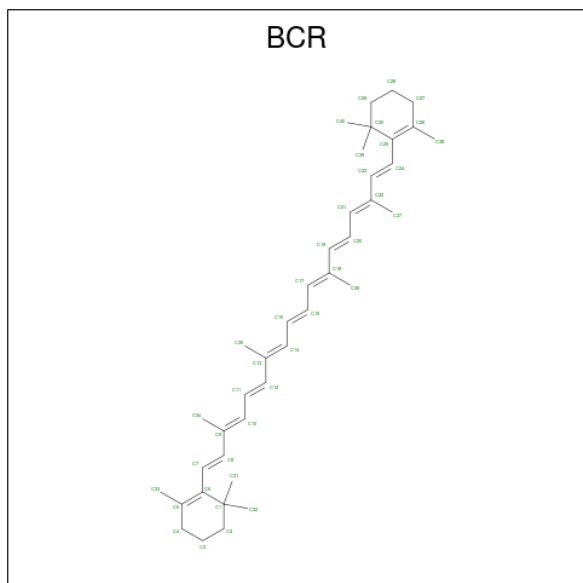
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
24	c	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
24	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	c	1	Total	C	H	Mg	N	O	0	0
			132	54	68	1	4	5		
24	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	h	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

- Molecule 25 is PHEOPHYTIN A (three-letter code: PHO) (formula: C₅₅H₇₄N₄O₅).



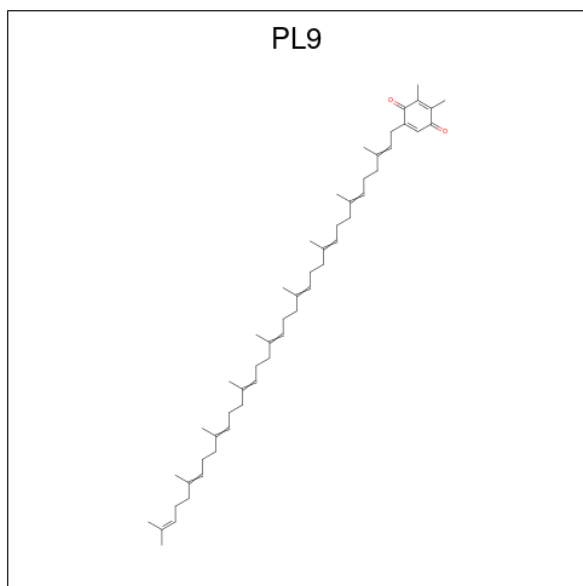
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
25	A	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
25	D	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
25	a	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
25	d	1	Total	C	H	N	O	0	0
			138	55	74	4	5		

- Molecule 26 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



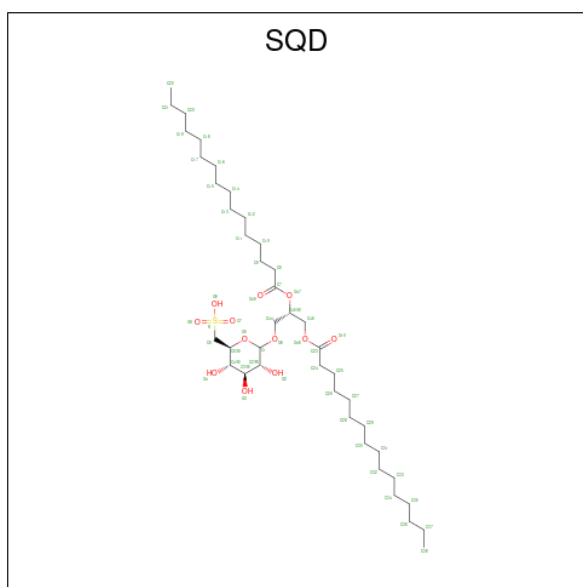
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	A	1	Total 96	C 40	H 56	0	0
26	B	1	Total 96	C 40	H 56	0	0
26	B	1	Total 96	C 40	H 56	0	0
26	B	1	Total 96	C 40	H 56	0	0
26	C	1	Total 96	C 40	H 56	0	0
26	C	1	Total 96	C 40	H 56	0	0
26	D	1	Total 96	C 40	H 56	0	0
26	H	1	Total 96	C 40	H 56	0	0
26	K	1	Total 96	C 40	H 56	0	0
26	Y	1	Total 96	C 40	H 56	0	0
26	a	1	Total 96	C 40	H 56	0	0
26	b	1	Total 96	C 40	H 56	0	0
26	b	1	Total 96	C 40	H 56	0	0
26	b	1	Total 96	C 40	H 56	0	0
26	b	1	Total 96	C 40	H 56	0	0
26	c	1	Total 96	C 40	H 56	0	0
26	c	1	Total 96	C 40	H 56	0	0
26	c	1	Total 96	C 40	H 56	0	0
26	d	1	Total 96	C 40	H 56	0	0
26	h	1	Total 96	C 40	H 56	0	0
26	k	1	Total 96	C 40	H 56	0	0
26	t	1	Total 96	C 40	H 56	0	0

- Molecule 27 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: $C_{53}H_{80}O_2$).



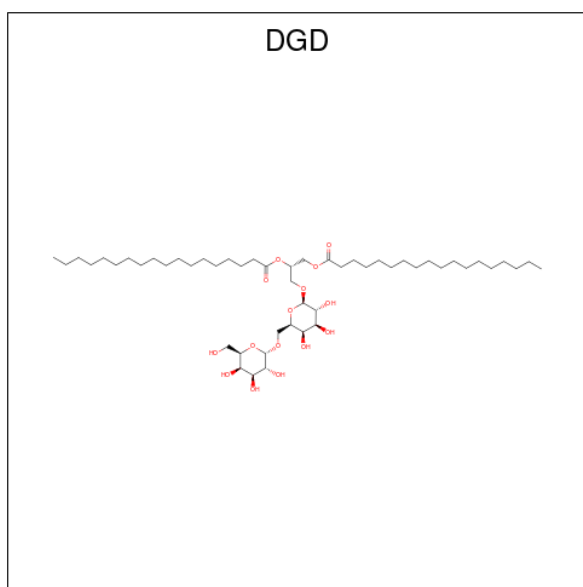
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
27	A	1	135	53	80	2	0	0
27	D	1	135	53	80	2	0	0
27	a	1	135	53	80	2	0	0
27	d	1	135	53	80	2	0	0

- Molecule 28 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



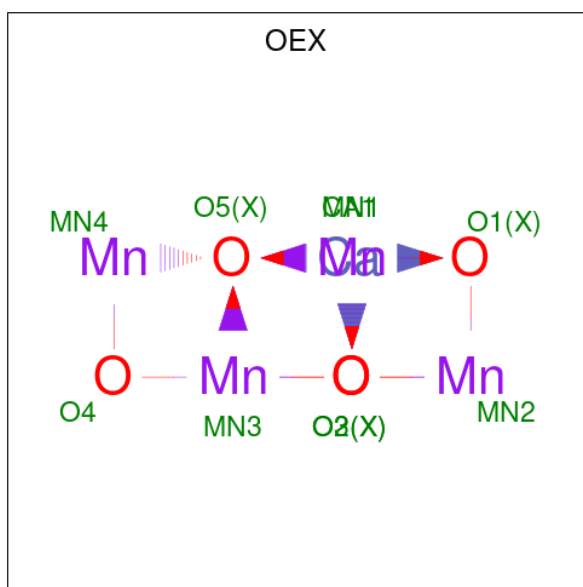
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	O	S		
28	A	1	122	39	70	12	1	0	0
28	A	1	104	35	65	4		0	0
28	B	1	132	41	78	12	1	0	0
28	F	1	81	25	45	10	1	0	0
28	a	1	132	41	78	12	1	0	0
28	a	1	92	31	56	5		0	0
28	b	1	114	36	65	12	1	0	0
28	f	1	90	28	49	12	1	0	0

- Molecule 29 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
29	A	1	Total 162	C 51	H 96	O 15	0	0
29	C	1	Total 144	C 47	H 82	O 15	0	0
29	C	1	Total 144	C 47	H 82	O 15	0	0
29	C	1	Total 144	C 47	H 82	O 15	0	0
29	H	1	Total 144	C 47	H 82	O 15	0	0
29	a	1	Total 119	C 39	H 75	O 5	0	0
29	c	1	Total 144	C 47	H 82	O 15	0	0
29	c	1	Total 144	C 47	H 82	O 15	0	0
29	c	1	Total 144	C 47	H 82	O 15	0	0
29	h	1	Total 144	C 47	H 82	O 15	0	0

- Molecule 30 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn_4O_5).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	Ca	Mn	O		
30	A	1	10	1	4	5	0	0
30	a	1	10	1	4	5	0	0

- Molecule 31 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

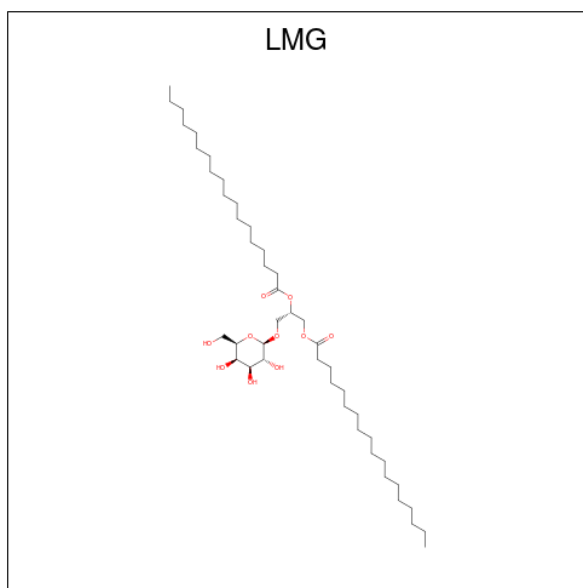
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
31	B	5	192	67	117	8	0	0
31	C	3	103	36	63	4	0	0
31	E	1	28	10	16	2	0	0
31	H	1	53	18	35		0	0
31	I	1	41	15	26		0	0
31	J	1	28	10	16	2	0	0
31	M	3	116	41	73	2	0	0
31	T	2	91	31	60		0	0
31	X	1	55	18	35	2	0	0
31	a	1	28	10	16	2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	b	4	Total	C	H	O	0	0
			176	60	110	6		
31	c	2	Total	C	H	O	0	0
			83	28	51	4		
31	d	1	Total	C	H	O	0	0
			43	15	26	2		
31	j	1	Total	C	H	O	0	0
			28	10	16	2		
31	m	1	Total	C	H	O	0	0
			28	10	16	2		
31	t	2	Total	C	H	O	0	0
			60	22	36	2		
31	x	1	Total	C	H	O	0	0
			55	18	35	2		

- Molecule 32 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



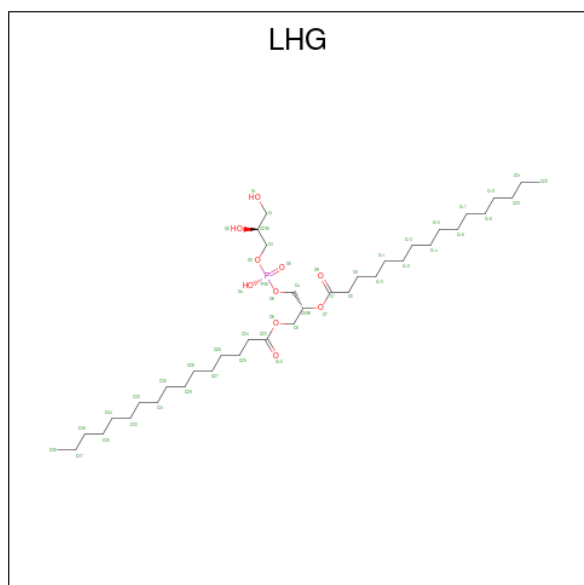
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	B	1	Total	C	H	O	0	0
			68	24	40	4		
32	C	1	Total	C	H	O	0	0
			114	38	66	10		
32	D	1	Total	C	H	O	0	0
			123	41	72	10		
32	D	1	Total	C	H	O	0	0
			78	27	45	6		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
32	K	1	Total 114	C 38	H 66	O 10	0	0
32	M	1	Total 123	C 41	H 72	O 10	0	0
32	b	1	Total 123	C 41	H 72	O 10	0	0
32	b	1	Total 141	C 45	H 86	O 10	0	0
32	c	1	Total 81	C 27	H 44	O 10	0	0
32	c	1	Total 117	C 38	H 69	O 10	0	0
32	c	1	Total 117	C 39	H 68	O 10	0	0
32	d	1	Total 102	C 34	H 58	O 10	0	0
32	h	1	Total 57	C 21	H 34	O 2	0	0

- Molecule 33 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{74}O_{10}P$).



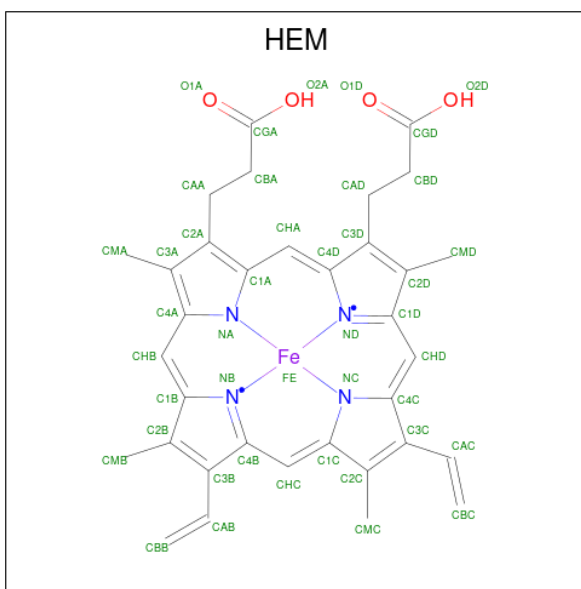
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	O	P		
33	D	1	Total 123	C 38	H 74	O 10	P 1	0	0
33	D	1	Total 114	C 36	H 67	O 10	P 1	0	0

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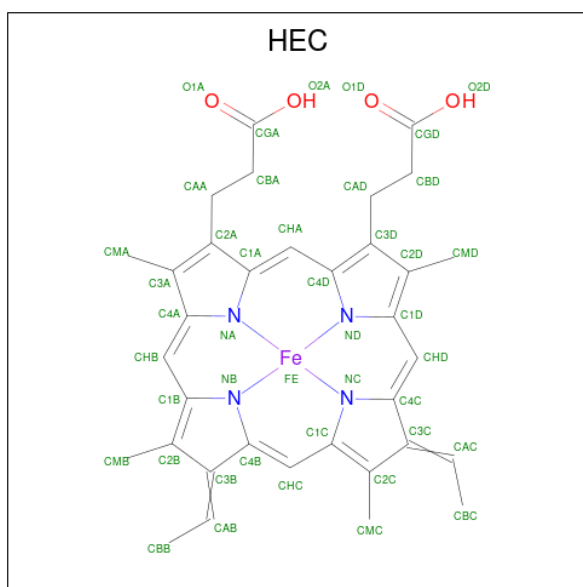
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
33	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	E	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	L	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	d	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	d	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	d	1	Total	C	H	O	P	0	0
			90	28	51	10	1		
33	e	1	Total	C	H	O	P	0	0
			99	31	57	10	1		
33	l	1	Total	C	H	O	P	0	0
			123	38	74	10	1		

- Molecule 34 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
34	F	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
34	e	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

- Molecule 35 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	Fe	H	N			O
35	V	1	73	34	1	30	4	4	0	0
35	v	1	73	34	1	30	4	4	0	0

- Molecule 36 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	A	141	Total 141	O 141	0	0
36	B	218	Total 218	O 218	0	0
36	C	197	Total 197	O 197	0	0
36	D	138	Total 138	O 138	0	0
36	E	29	Total 29	O 29	0	0
36	F	14	Total 14	O 14	0	0
36	H	26	Total 26	O 26	0	0
36	I	16	Total 16	O 16	0	0
36	J	12	Total 12	O 12	0	0
36	K	2	Total 2	O 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	L	9	Total O 9 9	0	0
36	M	5	Total O 5 5	0	0
36	O	125	Total O 125 125	0	0
36	T	11	Total O 11 11	0	0
36	U	52	Total O 52 52	0	0
36	V	68	Total O 68 68	0	0
36	Y	5	Total O 5 5	0	0
36	X	6	Total O 6 6	0	0
36	Z	3	Total O 3 3	0	0
36	R	4	Total O 4 4	0	0
36	a	121	Total O 121 121	0	0
36	b	187	Total O 187 187	0	0
36	c	156	Total O 156 156	0	0
36	d	123	Total O 123 123	0	0
36	e	22	Total O 22 22	0	0
36	f	2	Total O 2 2	0	0
36	h	19	Total O 19 19	0	0
36	i	10	Total O 10 10	0	0
36	j	10	Total O 10 10	0	0
36	k	5	Total O 5 5	0	0
36	l	9	Total O 9 9	0	0

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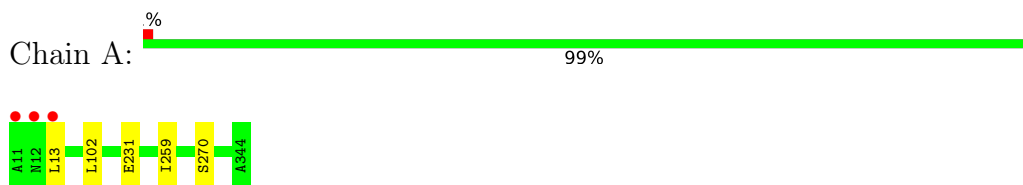
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	m	7	Total O 7 7	0	0
36	o	113	Total O 113 113	0	0
36	t	11	Total O 11 11	0	0
36	u	57	Total O 57 57	0	0
36	v	62	Total O 62 62	0	0
36	y	4	Total O 4 4	0	0
36	x	12	Total O 12 12	0	0
36	z	1	Total O 1 1	0	0
36	r	5	Total O 5 5	0	0

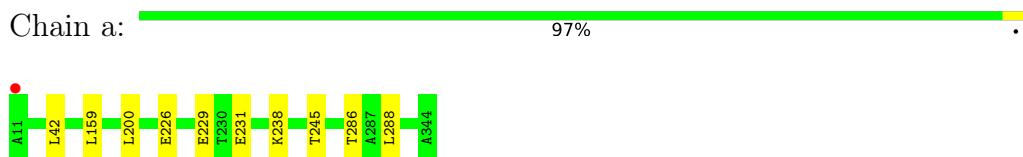
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

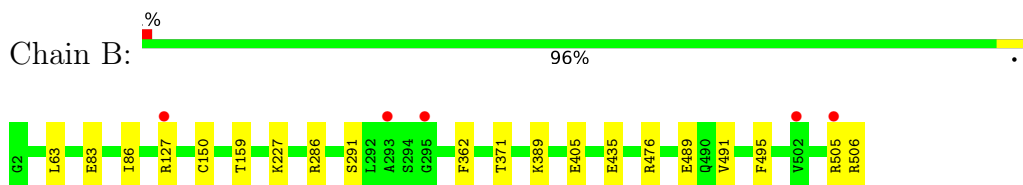
- Molecule 1: Photosystem II protein D1 1



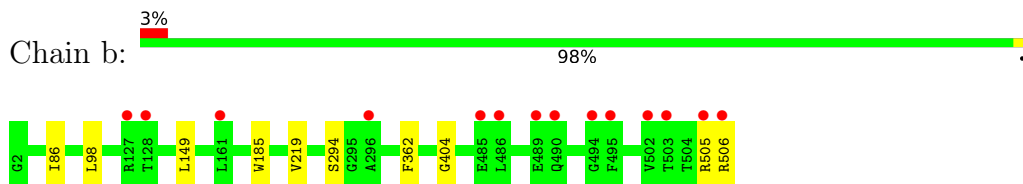
- Molecule 1: Photosystem II protein D1 1



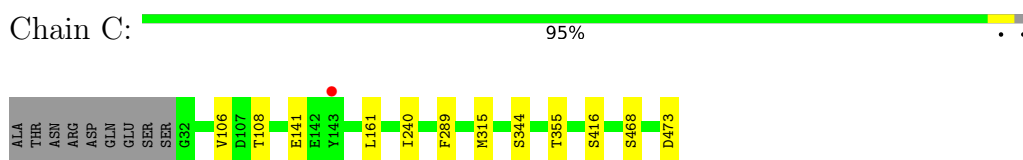
- Molecule 2: Photosystem II CP47 reaction center protein



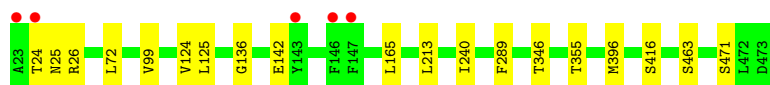
- Molecule 2: Photosystem II CP47 reaction center protein



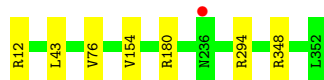
- Molecule 3: Photosystem II CP43 reaction center protein



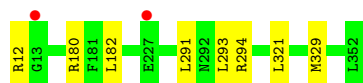
- Molecule 3: Photosystem II CP43 reaction center protein



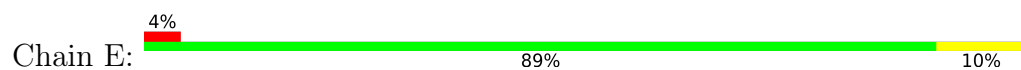
- Molecule 4: Photosystem II D2 protein



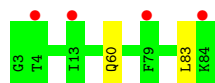
- Molecule 4: Photosystem II D2 protein



- Molecule 5: Cytochrome b559 subunit alpha



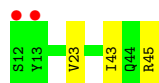
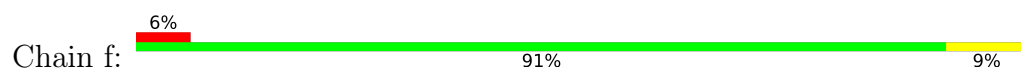
- Molecule 5: Cytochrome b559 subunit alpha



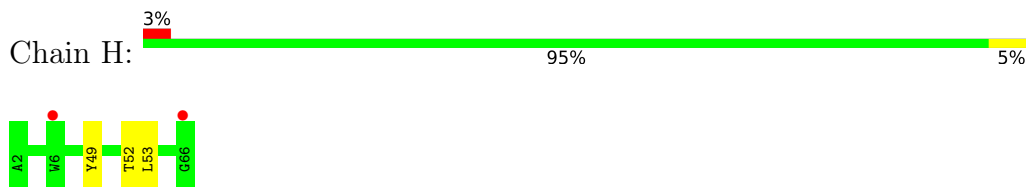
- Molecule 6: Cytochrome b559 subunit beta



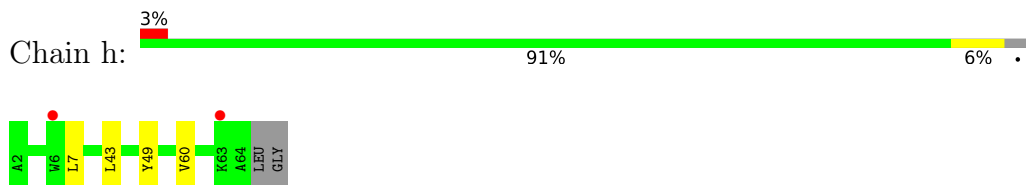
- Molecule 6: Cytochrome b559 subunit beta



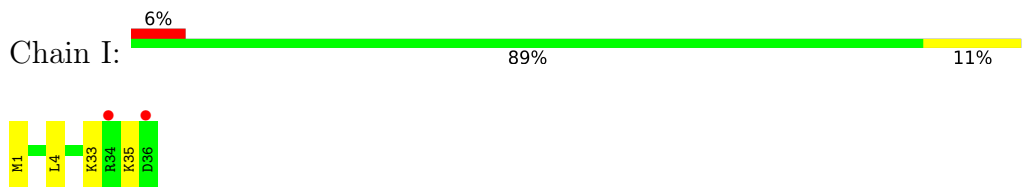
- Molecule 7: Photosystem II reaction center protein H



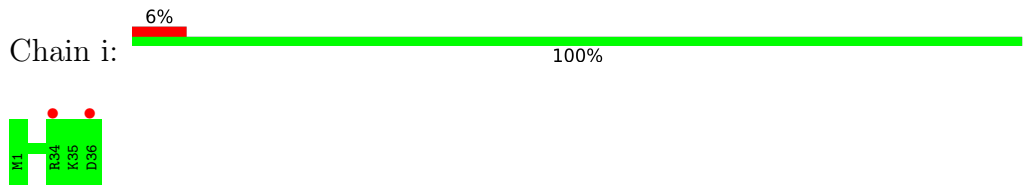
- Molecule 7: Photosystem II reaction center protein H



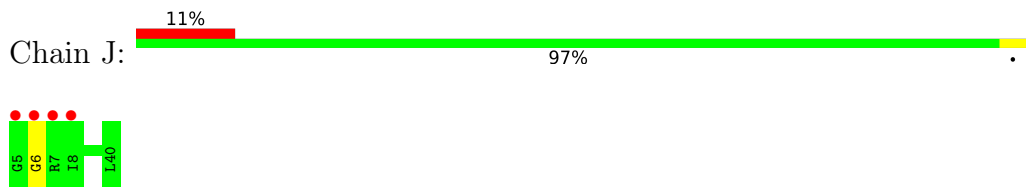
- Molecule 8: Photosystem II reaction center protein I



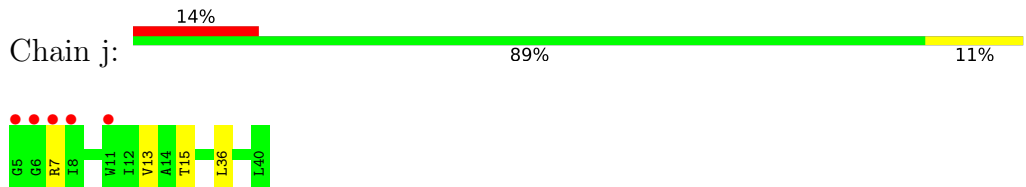
- Molecule 8: Photosystem II reaction center protein I



- Molecule 9: Photosystem II reaction center protein J



- Molecule 9: Photosystem II reaction center protein J

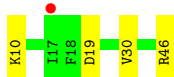
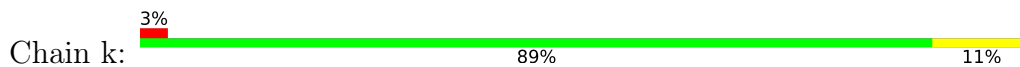


- Molecule 10: Photosystem II reaction center protein K





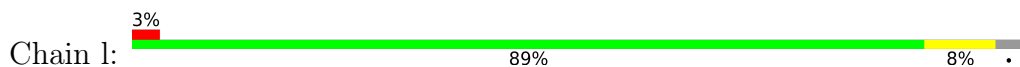
- Molecule 10: Photosystem II reaction center protein K



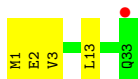
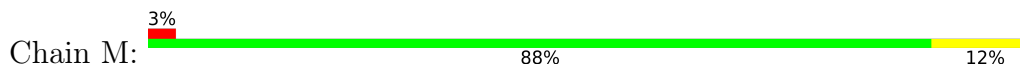
- Molecule 11: Photosystem II reaction center protein L



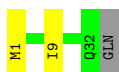
- Molecule 11: Photosystem II reaction center protein L



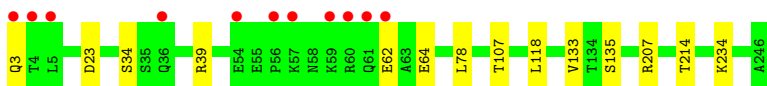
- Molecule 12: Photosystem II reaction center protein M



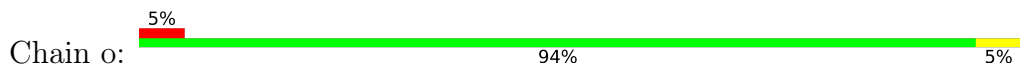
- Molecule 12: Photosystem II reaction center protein M

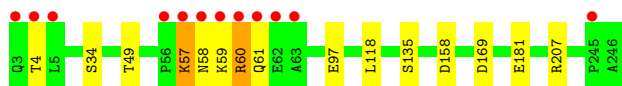


- Molecule 13: Photosystem II manganese-stabilizing polypeptide

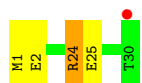
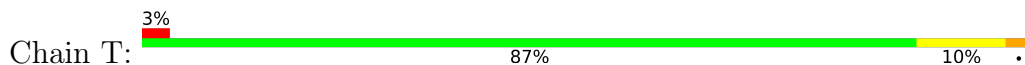


- Molecule 13: Photosystem II manganese-stabilizing polypeptide

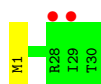




- Molecule 14: Photosystem II reaction center protein T



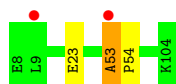
- Molecule 14: Photosystem II reaction center protein T



- Molecule 15: Photosystem II 12 kDa extrinsic protein



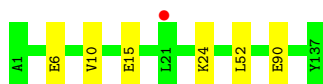
- Molecule 15: Photosystem II 12 kDa extrinsic protein



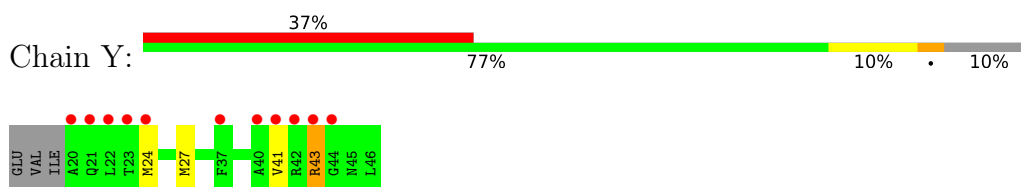
- Molecule 16: Cytochrome c-550



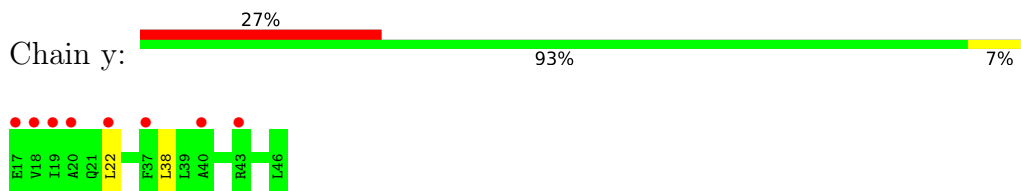
- Molecule 16: Cytochrome c-550



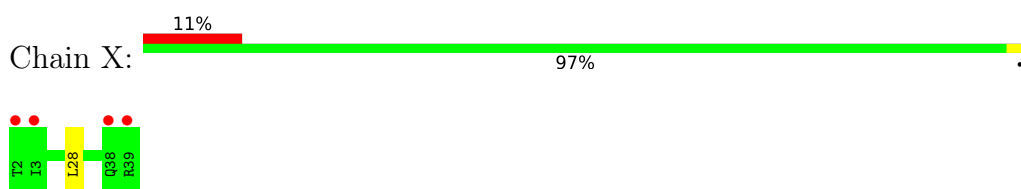
- Molecule 17: Photosystem II reaction center protein Ycf12



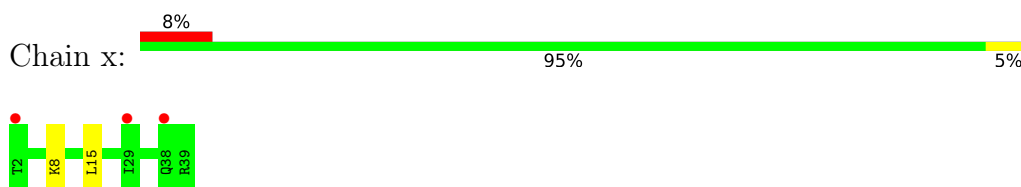
- Molecule 17: Photosystem II reaction center protein Ycf12



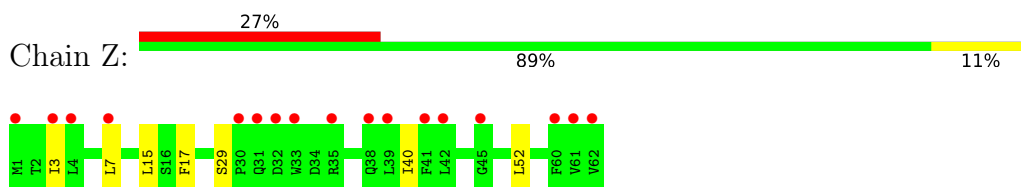
- Molecule 18: Photosystem II reaction center X protein



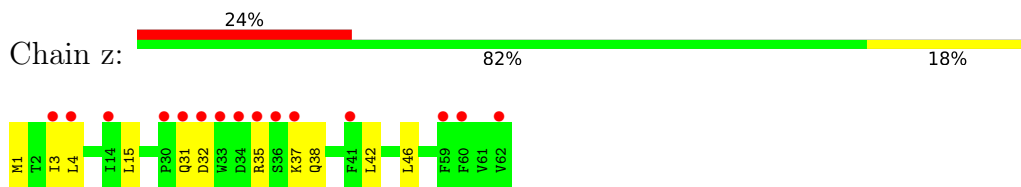
- Molecule 18: Photosystem II reaction center X protein



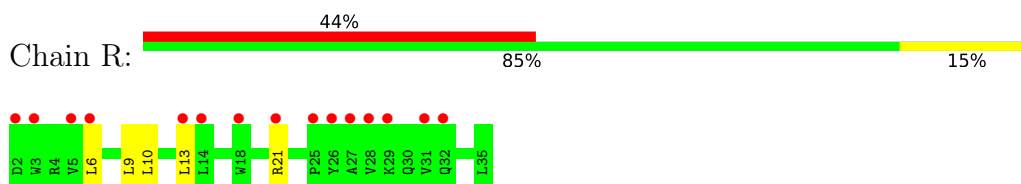
- Molecule 19: Photosystem II reaction center protein Z




- Molecule 19: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II protein Y



● Molecule 20: Photosystem II protein Y

Chain r:  62%
79% 12% 9%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	116.82Å 220.89Å 307.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.43 – 2.08 30.43 – 2.08	Depositor EDS
% Data completeness (in resolution range)	99.7 (30.43-2.08) 86.9 (30.43-2.08)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.56 (at 2.08Å)	Xtrriage
Refinement program	PHENIX dev_svn	Depositor
R, R_{free}	0.189 , 0.247 0.189 , 0.248	Depositor DCC
R_{free} test set	4194 reflections (0.89%)	wwPDB-VP
Wilson B-factor (Å ²)	27.1	Xtrriage
Anisotropy	0.298	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 72.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	103698	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LMG, HEM, LHG, FME, PL9, UNL, CLA, SQD, BCR, FE2, BCT, DGD, CL, PHO, OEX, HEC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.70	0/2707	0.72	0/3692
1	a	0.67	0/2704	0.71	0/3688
2	B	0.66	1/4160 (0.0%)	0.69	0/5668
2	b	0.64	1/4118 (0.0%)	0.67	0/5611
3	C	0.65	1/3538 (0.0%)	0.68	1/4818 (0.0%)
3	c	0.59	0/3619	0.67	0/4926
4	D	0.68	0/2812	0.71	2/3832 (0.1%)
4	d	0.62	0/2821	0.69	1/3844 (0.0%)
5	E	0.50	0/684	0.63	0/935
5	e	0.50	0/683	0.60	0/932
6	F	0.51	0/284	0.59	0/387
6	f	0.48	0/284	0.58	0/387
7	H	0.65	0/520	0.67	0/709
7	h	0.54	0/511	0.69	0/697
8	I	0.63	0/293	0.69	0/396
8	i	0.72	0/293	0.81	0/396
9	J	0.50	0/263	0.65	0/356
9	j	0.47	0/261	0.63	0/353
10	K	0.48	0/314	0.69	0/427
10	k	0.47	0/303	0.63	0/416
11	L	0.69	0/311	0.62	0/422
11	l	0.69	0/303	0.72	0/412
12	M	0.59	0/249	0.70	0/341
12	m	0.72	0/244	0.66	0/334
13	O	0.60	0/1914	0.73	0/2596
13	o	0.59	0/1905	0.74	2/2583 (0.1%)
14	T	0.68	0/257	0.89	2/349 (0.6%)
14	t	0.78	0/255	0.67	0/346
15	U	0.57	0/785	0.66	0/1064
15	u	0.64	0/785	0.72	0/1064
16	V	0.59	0/1085	0.68	0/1473
16	v	0.52	0/1085	0.66	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	Y	0.39	0/197	0.61	0/264
17	y	0.33	0/219	0.53	0/294
18	X	0.52	0/284	0.66	0/384
18	x	0.38	0/284	0.55	0/384
19	Z	0.53	0/490	0.59	0/669
19	z	0.41	0/488	0.54	0/666
20	R	0.43	0/277	0.59	0/380
20	r	0.38	0/233	0.53	0/323
All	All	0.62	3/42822 (0.0%)	0.68	8/58291 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
15	u	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	468	SER	C-N	-7.37	1.17	1.34
2	B	150	CYS	CB-SG	-5.50	1.72	1.81
2	b	185	TRP	CB-CG	-5.06	1.41	1.50

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	24	ARG	NE-CZ-NH1	7.73	124.17	120.30
4	d	294	ARG	NE-CZ-NH1	6.17	123.38	120.30
3	C	473	ASP	CB-CG-OD1	5.50	123.25	118.30
13	o	169	ASP	CB-CG-OD1	5.48	123.23	118.30
4	D	294	ARG	NE-CZ-NH1	-5.44	117.58	120.30
14	T	24	ARG	NE-CZ-NH2	-5.39	117.60	120.30
4	D	348	ARG	NE-CZ-NH2	-5.27	117.66	120.30
13	o	158	ASP	CB-CG-OD1	5.02	122.81	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	u	53	ALA	Peptide

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/334 (99%)	325 (98%)	6 (2%)	1 (0%)	41	39
1	a	332/334 (99%)	324 (98%)	8 (2%)	0	100	100
2	B	508/505 (101%)	494 (97%)	14 (3%)	0	100	100
2	b	503/505 (100%)	491 (98%)	10 (2%)	2 (0%)	34	31
3	C	441/451 (98%)	428 (97%)	12 (3%)	1 (0%)	47	47
3	c	451/451 (100%)	433 (96%)	15 (3%)	3 (1%)	22	17
4	D	339/341 (99%)	328 (97%)	11 (3%)	0	100	100
4	d	340/341 (100%)	325 (96%)	15 (4%)	0	100	100
5	E	80/82 (98%)	76 (95%)	4 (5%)	0	100	100
5	e	80/82 (98%)	77 (96%)	3 (4%)	0	100	100
6	F	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
6	f	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
7	H	63/65 (97%)	58 (92%)	5 (8%)	0	100	100
7	h	61/65 (94%)	55 (90%)	5 (8%)	1 (2%)	9	4
8	I	34/36 (94%)	32 (94%)	2 (6%)	0	100	100
8	i	34/36 (94%)	31 (91%)	3 (9%)	0	100	100
9	J	34/36 (94%)	31 (91%)	2 (6%)	1 (3%)	4	1
9	j	34/36 (94%)	31 (91%)	3 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	K	35/37 (95%)	34 (97%)	0	1 (3%)	4	1
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	34/37 (92%)	33 (97%)	1 (3%)	0	100	100
12	M	31/33 (94%)	31 (100%)	0	0	100	100
12	m	30/33 (91%)	29 (97%)	1 (3%)	0	100	100
13	O	243/244 (100%)	228 (94%)	13 (5%)	2 (1%)	19	14
13	o	242/244 (99%)	228 (94%)	11 (4%)	3 (1%)	13	7
14	T	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
14	t	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
15	U	95/97 (98%)	92 (97%)	3 (3%)	0	100	100
15	u	95/97 (98%)	89 (94%)	4 (4%)	2 (2%)	7	2
16	V	135/137 (98%)	130 (96%)	5 (4%)	0	100	100
16	v	135/137 (98%)	126 (93%)	9 (7%)	0	100	100
17	Y	25/30 (83%)	20 (80%)	3 (12%)	2 (8%)	1	0
17	y	28/30 (93%)	25 (89%)	3 (11%)	0	100	100
18	X	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
18	x	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	54 (90%)	6 (10%)	0	100	100
19	z	60/62 (97%)	53 (88%)	6 (10%)	1 (2%)	9	4
20	R	32/34 (94%)	30 (94%)	2 (6%)	0	100	100
20	r	29/34 (85%)	23 (79%)	5 (17%)	1 (3%)	3	1
All	All	5237/5326 (98%)	5019 (96%)	197 (4%)	21 (0%)	34	31

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
10	K	16	ALA
13	O	62	GLU
17	Y	41	VAL
3	c	416	SER
3	c	463	SER
13	o	60	ARG

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Mol	Chain	Res	Type
15	u	53	ALA
20	r	30	GLN
17	Y	43	ARG
13	o	57	LYS
13	o	61	GLN
19	z	15	LEU
2	b	505	ARG
15	u	54	PRO
2	b	404	GLY
13	O	133	VAL
7	h	60	VAL
9	J	6	GLY
1	A	259	ILE
3	c	136	GLY

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	270/270 (100%)	266 (98%)	4 (2%)	65 69
1	a	269/270 (100%)	259 (96%)	10 (4%)	34 34
2	B	407/403 (101%)	388 (95%)	19 (5%)	26 24
2	b	402/403 (100%)	395 (98%)	7 (2%)	60 65
3	C	345/352 (98%)	336 (97%)	9 (3%)	46 49
3	c	354/352 (101%)	338 (96%)	16 (4%)	27 26
4	D	276/276 (100%)	271 (98%)	5 (2%)	59 63
4	d	277/276 (100%)	270 (98%)	7 (2%)	47 50
5	E	72/72 (100%)	63 (88%)	9 (12%)	4 2
5	e	71/72 (99%)	69 (97%)	2 (3%)	43 46
6	F	28/28 (100%)	27 (96%)	1 (4%)	35 35
6	f	28/28 (100%)	25 (89%)	3 (11%)	6 3
7	H	53/54 (98%)	50 (94%)	3 (6%)	20 17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	h	53/54 (98%)	50 (94%)	3 (6%)	20	17
8	I	32/32 (100%)	29 (91%)	3 (9%)	8	5
8	i	32/32 (100%)	32 (100%)	0	100	100
9	J	24/24 (100%)	24 (100%)	0	100	100
9	j	23/24 (96%)	19 (83%)	4 (17%)	2	1
10	K	31/30 (103%)	29 (94%)	2 (6%)	17	13
10	k	30/30 (100%)	26 (87%)	4 (13%)	4	2
11	L	35/35 (100%)	33 (94%)	2 (6%)	20	17
11	l	34/35 (97%)	31 (91%)	3 (9%)	10	6
12	M	28/29 (97%)	25 (89%)	3 (11%)	6	3
12	m	28/29 (97%)	27 (96%)	1 (4%)	35	35
13	O	208/207 (100%)	196 (94%)	12 (6%)	20	16
13	o	207/207 (100%)	195 (94%)	12 (6%)	20	16
14	T	26/26 (100%)	23 (88%)	3 (12%)	5	3
14	t	25/26 (96%)	25 (100%)	0	100	100
15	U	84/84 (100%)	80 (95%)	4 (5%)	25	23
15	u	84/84 (100%)	83 (99%)	1 (1%)	71	76
16	V	117/117 (100%)	112 (96%)	5 (4%)	29	28
16	v	117/117 (100%)	111 (95%)	6 (5%)	24	21
17	Y	19/23 (83%)	16 (84%)	3 (16%)	2	1
17	y	22/23 (96%)	20 (91%)	2 (9%)	9	6
18	X	31/31 (100%)	30 (97%)	1 (3%)	39	40
18	x	31/31 (100%)	29 (94%)	2 (6%)	17	13
19	Z	52/52 (100%)	45 (86%)	7 (14%)	4	1
19	z	51/52 (98%)	41 (80%)	10 (20%)	1	0
20	R	28/29 (97%)	23 (82%)	5 (18%)	2	1
20	r	19/29 (66%)	16 (84%)	3 (16%)	2	1
All	All	4323/4348 (99%)	4127 (96%)	196 (4%)	27	26

All (196) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU

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Mol	Chain	Res	Type
1	A	102	LEU
1	A	231	GLU
1	A	270	SER
2	B	63	LEU
2	B	83	GLU
2	B	86	ILE
2	B	127	ARG
2	B	159	THR
2	B	227	LYS
2	B	286	ARG
2	B	291	SER
2	B	362	PHE
2	B	371	THR
2	B	389	LYS
2	B	405	GLU
2	B	435	GLU
2	B	476	ARG
2	B	489	GLU
2	B	491	VAL
2	B	495	PHE
2	B	505	ARG
2	B	506	ARG
3	C	106	VAL
3	C	108	THR
3	C	141	GLU
3	C	161	LEU
3	C	240	ILE
3	C	289	PHE
3	C	315	MET
3	C	344	SER
3	C	355	THR
4	D	12	ARG
4	D	43	LEU
4	D	76	VAL
4	D	154	VAL
4	D	180	ARG
5	E	4	THR
5	E	11	SER
5	E	22[A]	ILE
5	E	22[B]	ILE
5	E	65	LEU
5	E	71	GLU

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Mol	Chain	Res	Type
5	E	76	VAL
5	E	77	GLU
5	E	83	LEU
6	F	25	THR
7	H	49	TYR
7	H	52	THR
7	H	53	LEU
8	I	4	LEU
8	I	33	LYS
8	I	35	LYS
10	K	10	LYS
10	K	25	LEU
11	L	1	MET
11	L	2	GLU
12	M	2	GLU
12	M	3	VAL
12	M	13	LEU
13	O	3	GLN
13	O	23	ASP
13	O	34	SER
13	O	39	ARG
13	O	64	GLU
13	O	78	LEU
13	O	107	THR
13	O	118	LEU
13	O	135	SER
13	O	207	ARG
13	O	214	THR
13	O	234	LYS
14	T	2	GLU
14	T	24	ARG
14	T	25	GLU
15	U	39	ARG
15	U	59	GLU
15	U	67	LEU
15	U	86	GLU
16	V	3	LEU
16	V	7	VAL
16	V	14	SER
16	V	23	GLU
16	V	31	ARG
17	Y	24	MET

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Mol	Chain	Res	Type
17	Y	27	MET
17	Y	43	ARG
18	X	28	LEU
19	Z	3	ILE
19	Z	7	LEU
19	Z	15	LEU
19	Z	17	PHE
19	Z	29	SER
19	Z	40	ILE
19	Z	52	LEU
20	R	6	LEU
20	R	9	LEU
20	R	10	LEU
20	R	13	LEU
20	R	21	ARG
1	a	42	LEU
1	a	159	LEU
1	a	200	LEU
1	a	226	GLU
1	a	229	GLU
1	a	231	GLU
1	a	238	LYS
1	a	245	THR
1	a	286	THR
1	a	288	LEU
2	b	86	ILE
2	b	98	LEU
2	b	149	LEU
2	b	219	VAL
2	b	294	SER
2	b	362	PHE
2	b	506	ARG
3	c	24	THR
3	c	25	ASN
3	c	26	ARG
3	c	72	LEU
3	c	99	VAL
3	c	124	VAL
3	c	125	LEU
3	c	142	GLU
3	c	165	LEU
3	c	213	LEU

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Mol	Chain	Res	Type
3	c	240	ILE
3	c	289	PHE
3	c	346	THR
3	c	355	THR
3	c	396	MET
3	c	471	SER
4	d	12	ARG
4	d	180	ARG
4	d	182	LEU
4	d	291	LEU
4	d	293	LEU
4	d	321	LEU
4	d	329	MET
5	e	60	GLN
5	e	83	LEU
6	f	23	VAL
6	f	43	ILE
6	f	45	ARG
7	h	7	LEU
7	h	43	LEU
7	h	49	TYR
9	j	7	ARG
9	j	13	VAL
9	j	15	THR
9	j	36	LEU
10	k	10	LYS
10	k	19	ASP
10	k	30	VAL
10	k	46	ARG
11	l	11	GLU
11	l	21	LEU
11	l	30	LEU
12	m	9	ILE
13	o	4	THR
13	o	34	SER
13	o	49	THR
13	o	57	LYS
13	o	58	ASN
13	o	59	LYS
13	o	60	ARG
13	o	97	GLU
13	o	118	LEU

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Mol	Chain	Res	Type
13	o	135	SER
13	o	181	GLU
13	o	207	ARG
15	u	23	GLU
16	v	6	GLU
16	v	10	VAL
16	v	15	GLU
16	v	24	LYS
16	v	52	LEU
16	v	90	GLU
17	y	22	LEU
17	y	38	LEU
18	x	8	LYS
18	x	15	LEU
19	z	1	MET
19	z	3	ILE
19	z	4	LEU
19	z	31	GLN
19	z	32	ASP
19	z	35	ARG
19	z	37	LYS
19	z	38	GLN
19	z	42	LEU
19	z	46	LEU
20	r	3	TRP
20	r	13	LEU
20	r	22	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	289	GLN
13	O	82	GLN
13	O	88	ASN
17	Y	21	GLN
2	b	282	GLN
3	c	28	GLN
13	o	58	ASN
19	z	38	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

6 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	FME	T	1	14	8,9,10	1.05	1 (12%)	7,9,11	1.58	2 (28%)
14	FME	t	1	14	8,9,10	1.41	1 (12%)	7,9,11	1.36	1 (14%)
8	FME	I	1	8	8,9,10	0.97	0	7,9,11	1.66	1 (14%)
8	FME	i	1	8	8,9,10	1.12	0	7,9,11	0.90	0
12	FME	m	1	12	8,9,10	1.18	1 (12%)	7,9,11	0.84	0
12	FME	M	1	12	8,9,10	1.25	1 (12%)	7,9,11	1.09	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	FME	T	1	14	-	2/7/9/11	-
14	FME	t	1	14	-	1/7/9/11	-
8	FME	I	1	8	-	0/7/9/11	-
8	FME	i	1	8	-	1/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	t	1	FME	CA-N	-3.55	1.41	1.46
12	M	1	FME	CA-N	-2.84	1.42	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	m	1	FME	CA-N	-2.55	1.42	1.46
14	T	1	FME	CA-N	-2.27	1.43	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	1	FME	C-CA-N	3.97	116.89	109.73
14	T	1	FME	CA-N-CN	-2.56	118.89	122.82
14	t	1	FME	C-CA-N	2.46	114.18	109.73
14	T	1	FME	O1-CN-N	-2.23	119.39	125.27

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	M	1	FME	CB-CA-N-CN
14	T	1	FME	O-C-CA-CB
14	T	1	FME	CB-CG-SD-CE
14	t	1	FME	CB-CG-SD-CE
8	i	1	FME	CB-CA-N-CN

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 186 ligands modelled in this entry, 6 are monoatomic and 31 are unknown - leaving 149 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	LMG	c	522	-	48,48,55	1.19	6 (12%)	56,56,63	1.33	8 (14%)
29	DGD	c	517	-	63,63,67	1.23	9 (14%)	77,77,81	1.42	11 (14%)
24	CLA	C	514	-	65,73,73	1.44	7 (10%)	76,113,113	1.55	10 (13%)
24	CLA	C	504	-	65,73,73	1.64	12 (18%)	76,113,113	1.56	10 (13%)
24	CLA	C	506	-	65,73,73	1.48	10 (15%)	76,113,113	1.29	11 (14%)
26	BCR	b	618	-	41,41,41	1.16	3 (7%)	56,56,56	1.41	12 (21%)
27	PL9	D	406	-	55,55,55	1.85	9 (16%)	68,69,69	1.47	15 (22%)
24	CLA	B	611	-	65,73,73	1.42	6 (9%)	76,113,113	1.56	13 (17%)
24	CLA	c	506	-	65,73,73	2.20	11 (16%)	76,113,113	1.39	12 (15%)
33	LHG	E	101	-	48,48,48	0.91	3 (6%)	51,54,54	1.12	2 (3%)
24	CLA	b	615	-	65,73,73	1.58	9 (13%)	76,113,113	1.68	10 (13%)
33	LHG	D	411	-	48,48,48	1.03	6 (12%)	51,54,54	1.42	8 (15%)
29	DGD	c	516	-	63,63,67	1.11	3 (4%)	77,77,81	1.40	9 (11%)
24	CLA	B	610	36	65,73,73	1.82	11 (16%)	76,113,113	1.58	13 (17%)
26	BCR	b	620	-	41,41,41	1.11	2 (4%)	56,56,56	1.26	8 (14%)
24	CLA	B	603	-	65,73,73	1.46	8 (12%)	76,113,113	1.47	14 (18%)
24	CLA	C	505	36	59,67,73	1.41	6 (10%)	68,105,113	1.54	12 (17%)
26	BCR	h	103	-	41,41,41	1.13	1 (2%)	56,56,56	1.47	13 (23%)
32	LMG	K	102	-	48,48,55	1.05	4 (8%)	56,56,63	1.33	5 (8%)
24	CLA	C	511	-	65,73,73	1.54	9 (13%)	76,113,113	1.39	7 (9%)
28	SQD	A	412	-	38,38,54	1.08	3 (7%)	40,40,65	1.32	3 (7%)
29	DGD	a	412	-	43,43,67	1.20	3 (6%)	45,45,81	1.33	8 (17%)
24	CLA	B	608	-	65,73,73	1.52	11 (16%)	76,113,113	1.27	9 (11%)
26	BCR	b	602	-	41,41,41	1.15	3 (7%)	56,56,56	1.32	5 (8%)
35	HEC	v	201	16	32,50,50	2.27	7 (21%)	24,82,82	1.40	5 (20%)
24	CLA	b	610	-	65,73,73	1.50	6 (9%)	76,113,113	1.35	10 (13%)
24	CLA	c	503	-	65,73,73	1.66	7 (10%)	76,113,113	1.49	10 (13%)
24	CLA	c	505	-	65,73,73	1.52	8 (12%)	76,113,113	1.43	10 (13%)
24	CLA	c	512	-	65,73,73	1.49	8 (12%)	76,113,113	1.40	9 (11%)
24	CLA	D	403	-	65,73,73	1.49	13 (20%)	76,113,113	1.35	9 (11%)
25	PHO	A	407	-	51,69,69	1.08	5 (9%)	47,99,99	1.33	7 (14%)
24	CLA	c	507	36	65,73,73	1.46	11 (16%)	76,113,113	1.61	14 (18%)
27	PL9	A	410	-	55,55,55	1.39	4 (7%)	68,69,69	1.47	14 (20%)
28	SQD	A	411	-	51,52,54	1.02	4 (7%)	60,63,65	2.41	14 (23%)
24	CLA	D	402	36	65,73,73	1.66	9 (13%)	76,113,113	1.41	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	c	508	-	64,72,73	1.60	9 (14%)	74,111,113	1.20	6 (8%)
24	CLA	C	509	-	65,73,73	1.67	8 (12%)	76,113,113	1.63	12 (15%)
26	BCR	B	618	-	41,41,41	1.13	2 (4%)	56,56,56	1.33	7 (12%)
24	CLA	a	405	36	65,73,73	1.39	9 (13%)	76,113,113	1.34	8 (10%)
29	DGD	c	518	-	63,63,67	1.09	4 (6%)	77,77,81	1.42	11 (14%)
28	SQD	f	101	-	40,41,54	1.14	5 (12%)	49,52,65	1.67	8 (16%)
34	HEM	e	102	6,5	41,50,50	1.50	5 (12%)	45,82,82	1.43	7 (15%)
26	BCR	d	406	-	41,41,41	1.13	2 (4%)	56,56,56	1.23	6 (10%)
28	SQD	B	622	-	53,54,54	0.94	2 (3%)	62,65,65	1.85	13 (20%)
24	CLA	c	509	-	65,73,73	1.59	7 (10%)	76,113,113	1.56	12 (15%)
32	LMG	h	102	-	21,21,55	0.80	1 (4%)	20,20,63	1.01	1 (5%)
35	HEC	V	201	16	32,50,50	2.15	4 (12%)	24,82,82	1.29	2 (8%)
28	SQD	a	410	-	53,54,54	1.02	5 (9%)	62,65,65	2.02	13 (20%)
24	CLA	D	404	-	65,73,73	1.89	11 (16%)	76,113,113	1.02	5 (6%)
26	BCR	Y	101	-	41,41,41	1.08	2 (4%)	56,56,56	1.15	4 (7%)
33	LHG	D	408	-	48,48,48	1.05	5 (10%)	51,54,54	1.25	5 (9%)
28	SQD	F	101	-	35,36,54	1.01	3 (8%)	42,45,65	1.85	12 (28%)
32	LMG	D	407	-	51,51,55	1.13	5 (9%)	59,59,63	1.24	4 (6%)
32	LMG	d	411	-	44,44,55	1.07	3 (6%)	52,52,63	1.35	5 (9%)
30	OEX	a	414	36,3,1	0,15,15	-	-	-	-	-
24	CLA	c	501	-	65,73,73	1.63	10 (15%)	76,113,113	1.68	9 (11%)
24	CLA	A	408	-	54,62,73	1.76	11 (20%)	62,99,113	1.69	14 (22%)
25	PHO	d	402	-	51,69,69	1.11	6 (11%)	47,99,99	1.47	8 (17%)
24	CLA	B	604	-	65,73,73	1.64	8 (12%)	76,113,113	1.70	11 (14%)
33	LHG	d	408	-	48,48,48	0.71	0	51,54,54	1.22	5 (9%)
33	LHG	D	409	-	46,46,48	1.10	2 (4%)	49,52,54	1.40	7 (14%)
24	CLA	b	611	36	65,73,73	1.42	10 (15%)	76,113,113	1.47	14 (18%)
26	BCR	K	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.57	12 (21%)
24	CLA	b	605	-	65,73,73	1.55	9 (13%)	76,113,113	1.59	14 (18%)
28	SQD	a	411	-	35,35,54	1.10	2 (5%)	37,37,65	1.35	4 (10%)
24	CLA	a	407	-	65,73,73	1.71	11 (16%)	76,113,113	1.45	14 (18%)
24	CLA	c	511	3	65,73,73	1.98	8 (12%)	76,113,113	1.27	7 (9%)
24	CLA	A	406	36	65,73,73	1.44	12 (18%)	76,113,113	1.47	11 (14%)
24	CLA	B	609	-	65,73,73	1.61	10 (15%)	76,113,113	1.44	12 (15%)
32	LMG	c	519	-	37,37,55	1.10	3 (8%)	45,45,63	1.25	5 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	c	502	-	65,73,73	1.48	8 (12%)	76,113,113	1.40	10 (13%)
24	CLA	b	604	-	65,73,73	1.53	11 (16%)	76,113,113	1.63	15 (19%)
26	BCR	b	619	-	41,41,41	1.26	2 (4%)	56,56,56	1.46	11 (19%)
24	CLA	b	617	-	60,68,73	1.73	12 (20%)	70,107,113	1.67	10 (14%)
29	DGD	A	413	-	67,67,67	1.24	7 (10%)	81,81,81	1.49	10 (12%)
34	HEM	F	102	6,5	41,50,50	1.48	5 (12%)	45,82,82	1.28	4 (8%)
24	CLA	B	605	-	65,73,73	1.48	9 (13%)	76,113,113	1.57	13 (17%)
24	CLA	B	614	-	65,73,73	1.80	12 (18%)	76,113,113	1.24	6 (7%)
24	CLA	C	503	-	65,73,73	1.54	8 (12%)	76,113,113	1.62	11 (14%)
24	CLA	B	606	-	65,73,73	1.81	10 (15%)	76,113,113	1.46	10 (13%)
24	CLA	b	609	-	65,73,73	1.47	11 (16%)	76,113,113	1.45	13 (17%)
32	LMG	B	621	-	26,26,55	0.80	1 (3%)	26,26,63	1.17	2 (7%)
26	BCR	c	521	-	41,41,41	0.95	2 (4%)	56,56,56	1.24	7 (12%)
30	OEX	A	414	36,3,1	0,15,15	-	-	-	-	-
32	LMG	c	524	-	49,49,55	0.83	2 (4%)	57,57,63	1.36	4 (7%)
24	CLA	b	614	-	65,73,73	1.77	11 (16%)	76,113,113	1.47	12 (15%)
29	DGD	h	104	-	63,63,67	1.07	5 (7%)	77,77,81	1.39	8 (10%)
32	LMG	M	101	-	51,51,55	1.12	6 (11%)	59,59,63	1.58	14 (23%)
24	CLA	C	508	36	65,73,73	1.98	8 (12%)	76,113,113	1.45	7 (9%)
24	CLA	C	510	-	65,73,73	1.46	8 (12%)	76,113,113	1.30	7 (9%)
23	BCT	d	401	21	2,3,3	1.43	0	2,3,3	3.05	2 (100%)
26	BCR	a	408	-	41,41,41	1.19	3 (7%)	56,56,56	1.42	8 (14%)
33	LHG	d	409	-	48,48,48	0.71	0	51,54,54	1.24	5 (9%)
24	CLA	A	405	-	65,73,73	1.50	10 (15%)	76,113,113	1.40	10 (13%)
33	LHG	d	410	-	38,38,48	0.78	2 (5%)	41,44,54	1.15	3 (7%)
27	PL9	d	407	-	55,55,55	1.40	5 (9%)	68,69,69	1.82	22 (32%)
24	CLA	b	608	36	65,73,73	1.37	7 (10%)	76,113,113	1.39	7 (9%)
26	BCR	k	101	-	41,41,41	1.08	3 (7%)	56,56,56	1.12	3 (5%)
29	DGD	C	518	-	63,63,67	1.06	4 (6%)	77,77,81	1.48	13 (16%)
27	PL9	a	409	-	55,55,55	1.11	4 (7%)	68,69,69	1.48	12 (17%)
26	BCR	t	101	-	41,41,41	1.14	3 (7%)	56,56,56	1.39	8 (14%)
26	BCR	H	101	-	41,41,41	1.10	2 (4%)	56,56,56	1.28	8 (14%)
24	CLA	d	404	-	65,73,73	1.33	8 (12%)	76,113,113	1.42	9 (11%)
24	CLA	b	603	-	65,73,73	1.51	9 (13%)	76,113,113	1.67	12 (15%)
24	CLA	B	602	-	65,73,73	1.80	9 (13%)	76,113,113	1.39	12 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	SQD	b	601	-	48,49,54	0.96	2 (4%)	57,60,65	2.00	13 (22%)
32	LMG	D	410	-	31,31,55	1.15	3 (9%)	33,33,63	1.08	0
24	CLA	b	606	-	65,73,73	1.53	8 (12%)	76,113,113	1.58	14 (18%)
24	CLA	b	616	-	65,73,73	1.78	11 (16%)	76,113,113	1.57	9 (11%)
24	CLA	C	512	3	65,73,73	1.63	12 (18%)	76,113,113	1.58	8 (10%)
26	BCR	A	409	-	41,41,41	1.06	3 (7%)	56,56,56	1.30	7 (12%)
26	BCR	C	519	-	41,41,41	1.05	2 (4%)	56,56,56	1.38	9 (16%)
33	LHG	L	101	-	48,48,48	0.68	1 (2%)	51,54,54	1.17	3 (5%)
26	BCR	c	514	-	41,41,41	1.19	2 (4%)	56,56,56	1.34	9 (16%)
24	CLA	B	601	36	65,73,73	1.98	9 (13%)	76,113,113	1.51	9 (11%)
24	CLA	c	510	-	65,73,73	1.63	7 (10%)	76,113,113	1.54	8 (10%)
24	CLA	B	616	-	60,68,73	1.79	12 (20%)	70,107,113	1.48	11 (15%)
24	CLA	b	613	-	65,73,73	1.56	7 (10%)	76,113,113	1.55	11 (14%)
26	BCR	c	515	-	41,41,41	1.35	4 (9%)	56,56,56	1.42	11 (19%)
25	PHO	a	406	-	51,69,69	1.15	5 (9%)	47,99,99	1.29	6 (12%)
29	DGD	C	517	-	63,63,67	1.15	6 (9%)	77,77,81	1.46	13 (16%)
33	LHG	l	101	-	48,48,48	0.84	1 (2%)	51,54,54	1.26	7 (13%)
29	DGD	C	516	-	63,63,67	1.19	6 (9%)	77,77,81	1.33	12 (15%)
32	LMG	C	501	-	48,48,55	0.90	1 (2%)	56,56,63	1.38	9 (16%)
24	CLA	h	101	36	65,73,73	1.80	11 (16%)	76,113,113	1.49	14 (18%)
24	CLA	b	612	-	65,73,73	1.71	11 (16%)	76,113,113	1.39	11 (14%)
25	PHO	D	401	-	51,69,69	1.13	5 (9%)	47,99,99	1.38	5 (10%)
24	CLA	C	502	-	65,73,73	1.90	11 (16%)	76,113,113	1.43	9 (11%)
26	BCR	D	405	-	41,41,41	1.06	2 (4%)	56,56,56	1.15	3 (5%)
24	CLA	B	607	36	65,73,73	1.49	8 (12%)	76,113,113	1.48	11 (14%)
29	DGD	H	102	-	63,63,67	1.28	9 (14%)	77,77,81	1.45	9 (11%)
33	LHG	e	101	-	41,41,48	0.75	0	44,47,54	1.30	3 (6%)
32	LMG	b	623	-	55,55,55	0.95	5 (9%)	63,63,63	1.42	7 (11%)
24	CLA	B	612	-	65,73,73	1.31	6 (9%)	76,113,113	1.42	10 (13%)
24	CLA	c	513	-	65,73,73	1.57	9 (13%)	76,113,113	1.17	8 (10%)
24	CLA	c	504	36	60,68,73	1.59	10 (16%)	70,107,113	1.51	10 (14%)
24	CLA	B	613	-	65,73,73	1.73	12 (18%)	76,113,113	1.60	11 (14%)
24	CLA	C	507	-	65,73,73	1.72	9 (13%)	76,113,113	1.27	7 (9%)
24	CLA	d	403	36	65,73,73	1.57	9 (13%)	76,113,113	1.58	13 (17%)
26	BCR	B	617	-	41,41,41	1.20	3 (7%)	56,56,56	1.46	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	LMG	b	621	-	51,51,55	0.82	0	59,59,63	1.52	10 (16%)
23	BCT	A	404	21	2,3,3	1.20	0	2,3,3	3.23	1 (50%)
26	BCR	B	619	-	41,41,41	1.25	2 (4%)	56,56,56	1.51	12 (21%)
24	CLA	a	404	-	65,73,73	1.54	10 (15%)	76,113,113	1.59	11 (14%)
24	CLA	b	607	-	65,73,73	2.03	9 (13%)	76,113,113	1.66	16 (21%)
24	CLA	d	405	-	65,73,73	1.83	9 (13%)	76,113,113	1.60	16 (21%)
24	CLA	C	513	-	65,73,73	1.48	10 (15%)	76,113,113	1.42	11 (14%)
26	BCR	C	515	-	41,41,41	1.41	4 (9%)	56,56,56	1.36	9 (16%)
24	CLA	B	615	-	65,73,73	1.63	11 (16%)	76,113,113	1.47	9 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	LMG	c	522	-	-	24/43/63/70	0/1/1/1
29	DGD	c	517	-	-	15/51/91/95	0/2/2/2
24	CLA	C	514	-	1/1/20/20	10/37/115/115	-
24	CLA	C	504	-	1/1/20/20	5/37/115/115	-
24	CLA	C	506	-	1/1/20/20	11/37/115/115	-
26	BCR	b	618	-	-	6/29/63/63	0/2/2/2
27	PL9	D	406	-	-	10/53/73/73	0/1/1/1
24	CLA	c	506	-	1/1/20/20	19/37/115/115	-
24	CLA	B	611	-	-	10/37/115/115	-
33	LHG	E	101	-	-	26/53/53/53	-
24	CLA	b	615	-	1/1/20/20	15/37/115/115	-
33	LHG	D	411	-	-	16/53/53/53	-
29	DGD	c	516	-	-	26/51/91/95	0/2/2/2
24	CLA	B	610	36	1/1/20/20	5/37/115/115	-
26	BCR	b	620	-	-	8/29/63/63	0/2/2/2
24	CLA	C	505	36	1/1/18/20	9/30/108/115	-
24	CLA	B	603	-	-	11/37/115/115	-
26	BCR	h	103	-	-	10/29/63/63	0/2/2/2
32	LMG	K	102	-	-	10/43/63/70	0/1/1/1
24	CLA	C	511	-	1/1/20/20	14/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	SQD	A	412	-	-	17/39/39/69	-
29	DGD	a	412	-	-	21/45/45/95	-
24	CLA	B	608	-	-	5/37/115/115	-
26	BCR	b	602	-	-	11/29/63/63	0/2/2/2
35	HEC	v	201	16	-	2/10/54/54	-
24	CLA	b	610	-	1/1/20/20	12/37/115/115	-
24	CLA	c	503	-	1/1/20/20	8/37/115/115	-
24	CLA	c	505	-	1/1/20/20	9/37/115/115	-
24	CLA	c	512	-	1/1/20/20	20/37/115/115	-
24	CLA	D	403	-	1/1/20/20	7/37/115/115	-
25	PHO	A	407	-	-	6/37/103/103	0/5/6/6
24	CLA	c	507	36	1/1/20/20	9/37/115/115	-
27	PL9	A	410	-	-	24/53/73/73	0/1/1/1
28	SQD	A	411	-	-	23/47/67/69	0/1/1/1
24	CLA	D	402	36	1/1/20/20	3/37/115/115	-
24	CLA	c	508	-	-	9/36/114/115	-
24	CLA	C	509	-	-	11/37/115/115	-
26	BCR	B	618	-	-	3/29/63/63	0/2/2/2
24	CLA	a	405	36	-	13/37/115/115	-
29	DGD	c	518	-	-	16/51/91/95	0/2/2/2
28	SQD	f	101	-	-	18/36/56/69	0/1/1/1
34	HEM	e	102	6,5	-	4/12/54/54	-
26	BCR	d	406	-	-	11/29/63/63	0/2/2/2
28	SQD	B	622	-	-	22/49/69/69	0/1/1/1
24	CLA	c	509	-	1/1/20/20	16/37/115/115	-
32	LMG	h	102	-	-	13/17/17/70	-
35	HEC	V	201	16	-	2/10/54/54	-
28	SQD	a	410	-	-	23/49/69/69	0/1/1/1
24	CLA	D	404	-	-	10/37/115/115	-
26	BCR	Y	101	-	-	6/29/63/63	0/2/2/2
33	LHG	D	408	-	-	21/53/53/53	-
28	SQD	F	101	-	-	13/28/48/69	0/1/1/1
32	LMG	D	407	-	-	17/46/66/70	0/1/1/1
32	LMG	d	411	-	-	11/39/59/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	c	501	-	1/1/20/20	6/37/115/115	-
24	CLA	A	408	-	1/1/17/20	4/24/102/115	-
25	PHO	d	402	-	-	6/37/103/103	0/5/6/6
24	CLA	B	604	-	1/1/20/20	13/37/115/115	-
33	LHG	d	408	-	-	21/53/53/53	-
33	LHG	D	409	-	-	25/51/51/53	-
24	CLA	b	611	36	1/1/20/20	9/37/115/115	-
26	BCR	K	101	-	-	11/29/63/63	0/2/2/2
24	CLA	b	605	-	1/1/20/20	11/37/115/115	-
28	SQD	a	411	-	-	23/37/37/69	-
24	CLA	a	407	-	1/1/20/20	8/37/115/115	-
24	CLA	c	511	3	1/1/20/20	6/37/115/115	-
24	CLA	A	406	36	1/1/20/20	6/37/115/115	-
24	CLA	B	609	-	-	5/37/115/115	-
32	LMG	c	519	-	-	13/31/51/70	0/1/1/1
24	CLA	c	502	-	1/1/20/20	4/37/115/115	-
24	CLA	b	604	-	1/1/20/20	8/37/115/115	-
26	BCR	b	619	-	-	5/29/63/63	0/2/2/2
24	CLA	b	617	-	1/1/19/20	8/31/109/115	-
29	DGD	A	413	-	-	25/55/95/95	0/2/2/2
34	HEM	F	102	6,5	-	2/12/54/54	-
24	CLA	B	605	-	1/1/20/20	12/37/115/115	-
24	CLA	B	614	-	1/1/20/20	11/37/115/115	-
24	CLA	C	503	-	1/1/20/20	13/37/115/115	-
24	CLA	B	606	-	1/1/20/20	6/37/115/115	-
24	CLA	b	609	-	1/1/20/20	5/37/115/115	-
32	LMG	B	621	-	-	8/22/22/70	-
26	BCR	c	521	-	-	14/29/63/63	0/2/2/2
32	LMG	c	524	-	-	25/44/64/70	0/1/1/1
24	CLA	b	614	-	1/1/20/20	7/37/115/115	-
29	DGD	h	104	-	-	18/51/91/95	0/2/2/2
32	LMG	M	101	-	-	21/46/66/70	0/1/1/1
24	CLA	C	508	36	1/1/20/20	7/37/115/115	-
24	CLA	C	510	-	1/1/20/20	10/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	a	408	-	-	3/29/63/63	0/2/2/2
33	LHG	d	409	-	-	18/53/53/53	-
24	CLA	A	405	-	1/1/20/20	3/37/115/115	-
33	LHG	d	410	-	-	11/43/43/53	-
27	PL9	d	407	-	-	17/53/73/73	0/1/1/1
24	CLA	b	608	36	1/1/20/20	14/37/115/115	-
26	BCR	k	101	-	-	10/29/63/63	0/2/2/2
29	DGD	C	518	-	-	14/51/91/95	0/2/2/2
27	PL9	a	409	-	-	22/53/73/73	0/1/1/1
26	BCR	t	101	-	-	12/29/63/63	0/2/2/2
26	BCR	H	101	-	-	7/29/63/63	0/2/2/2
24	CLA	d	404	-	1/1/20/20	7/37/115/115	-
24	CLA	b	603	-	1/1/20/20	9/37/115/115	-
24	CLA	B	602	-	1/1/20/20	6/37/115/115	-
28	SQD	b	601	-	-	21/44/64/69	0/1/1/1
32	LMG	D	410	-	-	19/33/33/70	-
24	CLA	b	606	-	1/1/20/20	10/37/115/115	-
24	CLA	b	616	-	1/1/20/20	9/37/115/115	-
24	CLA	C	512	3	1/1/20/20	10/37/115/115	-
26	BCR	A	409	-	-	8/29/63/63	0/2/2/2
26	BCR	C	519	-	-	11/29/63/63	0/2/2/2
33	LHG	L	101	-	-	22/53/53/53	-
26	BCR	c	514	-	-	10/29/63/63	0/2/2/2
24	CLA	B	601	36	1/1/20/20	12/37/115/115	-
24	CLA	c	510	-	1/1/20/20	17/37/115/115	-
24	CLA	B	616	-	1/1/19/20	10/31/109/115	-
24	CLA	b	613	-	1/1/20/20	5/37/115/115	-
26	BCR	c	515	-	-	8/29/63/63	0/2/2/2
25	PHO	a	406	-	-	3/37/103/103	0/5/6/6
29	DGD	C	517	-	-	20/51/91/95	0/2/2/2
33	LHG	l	101	-	-	18/53/53/53	-
29	DGD	C	516	-	-	18/51/91/95	0/2/2/2
32	LMG	C	501	-	-	24/43/63/70	0/1/1/1
24	CLA	h	101	36	1/1/20/20	19/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	b	612	-	1/1/20/20	7/37/115/115	-
25	PHO	D	401	-	-	2/37/103/103	0/5/6/6
24	CLA	C	502	-	1/1/20/20	2/37/115/115	-
26	BCR	D	405	-	-	5/29/63/63	0/2/2/2
24	CLA	B	607	36	1/1/20/20	12/37/115/115	-
29	DGD	H	102	-	-	17/51/91/95	0/2/2/2
33	LHG	e	101	-	-	29/46/46/53	-
32	LMG	b	623	-	-	18/50/70/70	0/1/1/1
24	CLA	B	612	-	1/1/20/20	14/37/115/115	-
24	CLA	c	513	-	1/1/20/20	11/37/115/115	-
24	CLA	c	504	36	1/1/19/20	8/31/109/115	-
24	CLA	B	613	-	1/1/20/20	11/37/115/115	-
24	CLA	d	403	36	1/1/20/20	3/37/115/115	-
24	CLA	C	507	-	-	13/37/115/115	-
26	BCR	B	617	-	-	5/29/63/63	0/2/2/2
32	LMG	b	621	-	-	21/46/66/70	0/1/1/1
26	BCR	B	619	-	-	7/29/63/63	0/2/2/2
24	CLA	a	404	-	1/1/20/20	6/37/115/115	-
24	CLA	b	607	-	1/1/20/20	11/37/115/115	-
24	CLA	d	405	-	1/1/20/20	4/37/115/115	-
24	CLA	C	513	-	1/1/20/20	12/37/115/115	-
26	BCR	C	515	-	-	2/29/63/63	0/2/2/2
24	CLA	B	615	-	1/1/20/20	11/37/115/115	-

All (917) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	506	CLA	MG-ND	-12.77	1.80	2.05
24	C	508	CLA	MG-NA	10.07	2.30	2.06
24	b	607	CLA	MG-NA	9.96	2.29	2.06
24	B	602	CLA	C4B-NB	9.47	1.43	1.35
24	c	511	CLA	C4B-NB	9.25	1.43	1.35
24	B	610	CLA	C4B-NB	9.10	1.43	1.35
24	B	601	CLA	MG-NA	9.03	2.27	2.06
24	B	601	CLA	C4B-NB	8.88	1.43	1.35
24	b	614	CLA	C4B-NB	8.60	1.42	1.35
24	B	613	CLA	C4B-NB	8.41	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	502	CLA	C4B-NB	8.21	1.42	1.35
24	c	511	CLA	MG-NA	8.19	2.25	2.06
24	h	101	CLA	C4B-NB	8.06	1.42	1.35
24	b	610	CLA	C4B-NB	7.87	1.42	1.35
24	b	617	CLA	C4B-NB	7.85	1.42	1.35
24	B	614	CLA	C4B-NB	7.73	1.42	1.35
35	v	201	HEC	C2B-C3B	-7.64	1.32	1.40
24	c	510	CLA	C4B-NB	7.58	1.42	1.35
24	b	607	CLA	C4B-NB	7.56	1.42	1.35
24	b	615	CLA	C4B-NB	7.51	1.41	1.35
24	d	405	CLA	C4B-NB	7.49	1.41	1.35
24	C	508	CLA	C4B-NB	7.48	1.41	1.35
35	V	201	HEC	C2B-C3B	-7.46	1.33	1.40
24	c	504	CLA	C4B-NB	7.38	1.41	1.35
24	D	402	CLA	C4B-NB	7.38	1.41	1.35
24	c	512	CLA	C4B-NB	7.33	1.41	1.35
24	b	606	CLA	C4B-NB	7.32	1.41	1.35
24	B	615	CLA	C4B-NB	7.30	1.41	1.35
24	c	503	CLA	C4B-NB	7.27	1.41	1.35
24	B	609	CLA	C4B-NB	7.14	1.41	1.35
24	C	502	CLA	MG-ND	-7.13	1.91	2.05
24	b	605	CLA	C4B-NB	7.12	1.41	1.35
24	c	508	CLA	C4B-NB	7.02	1.41	1.35
24	A	408	CLA	C4B-NB	6.99	1.41	1.35
24	c	501	CLA	C4B-NB	6.99	1.41	1.35
24	c	513	CLA	C4B-NB	6.92	1.41	1.35
24	D	404	CLA	C4B-NB	6.90	1.41	1.35
24	B	616	CLA	MG-NA	6.84	2.22	2.06
24	b	616	CLA	C4B-NB	6.83	1.41	1.35
24	B	616	CLA	C4B-NB	6.82	1.41	1.35
24	B	611	CLA	C4B-NB	6.79	1.41	1.35
24	d	405	CLA	MG-NA	6.78	2.22	2.06
24	b	603	CLA	C4B-NB	6.72	1.41	1.35
27	D	406	PL9	C6-C1	-6.71	1.36	1.48
24	B	606	CLA	MG-NA	6.66	2.22	2.06
24	B	606	CLA	C4B-NB	6.63	1.41	1.35
24	a	404	CLA	C4B-NB	6.61	1.41	1.35
24	b	612	CLA	MG-NC	-6.47	1.90	2.06
24	C	511	CLA	C4B-NB	6.45	1.41	1.35
24	C	507	CLA	MG-ND	-6.44	1.93	2.05
24	C	504	CLA	C4B-NB	6.43	1.40	1.35
24	C	506	CLA	C4B-NB	6.40	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	604	CLA	C4B-NB	6.40	1.40	1.35
24	b	604	CLA	C4B-NB	6.39	1.40	1.35
24	C	507	CLA	C4B-NB	6.34	1.40	1.35
24	a	407	CLA	C4B-NB	6.27	1.40	1.35
24	b	616	CLA	MG-NA	6.26	2.21	2.06
24	C	510	CLA	C4B-NB	6.25	1.40	1.35
24	b	608	CLA	C4B-NB	6.22	1.40	1.35
24	C	505	CLA	C4B-NB	6.19	1.40	1.35
24	c	506	CLA	C4B-NB	6.18	1.40	1.35
24	C	512	CLA	C4B-NB	6.17	1.40	1.35
24	B	603	CLA	C4B-NB	6.13	1.40	1.35
24	D	404	CLA	MG-ND	-6.13	1.93	2.05
24	C	514	CLA	C4B-NB	6.13	1.40	1.35
24	C	509	CLA	MG-ND	6.11	2.17	2.05
24	h	101	CLA	MG-NA	6.06	2.20	2.06
24	b	613	CLA	MG-ND	-6.02	1.93	2.05
27	D	406	PL9	C3-C4	-6.02	1.39	1.49
24	c	509	CLA	C4B-NB	5.98	1.40	1.35
35	v	201	HEC	C3C-C2C	-5.95	1.34	1.40
24	b	612	CLA	MG-NA	5.94	2.20	2.06
24	A	405	CLA	C4B-NB	5.80	1.40	1.35
24	c	509	CLA	MG-ND	5.73	2.17	2.05
24	B	613	CLA	MG-NA	5.71	2.19	2.06
24	a	407	CLA	MG-ND	-5.71	1.94	2.05
24	c	507	CLA	C4B-NB	5.70	1.40	1.35
24	d	403	CLA	MG-ND	5.69	2.17	2.05
24	C	512	CLA	MG-NA	5.68	2.19	2.06
24	C	513	CLA	C4B-NB	5.68	1.40	1.35
24	B	614	CLA	MG-NC	-5.65	1.92	2.06
24	B	614	CLA	MG-ND	-5.62	1.94	2.05
35	V	201	HEC	C3C-C2C	-5.61	1.34	1.40
24	c	505	CLA	C4B-NB	5.60	1.40	1.35
26	C	515	BCR	C1-C6	-5.52	1.46	1.53
24	c	503	CLA	MG-NC	5.39	2.19	2.06
24	C	503	CLA	C4B-NB	5.36	1.40	1.35
24	D	402	CLA	C4D-ND	-5.34	1.30	1.37
24	D	404	CLA	MG-NC	5.30	2.18	2.06
24	c	510	CLA	MG-ND	-5.27	1.95	2.05
24	D	404	CLA	C3B-C2B	-5.26	1.33	1.40
27	D	406	PL9	C11-C9	-5.26	1.40	1.51
24	B	612	CLA	C4D-ND	-5.25	1.30	1.37
24	C	509	CLA	C4B-NB	5.24	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	614	CLA	MG-NA	5.24	2.18	2.06
24	c	501	CLA	MG-NA	5.23	2.18	2.06
24	C	504	CLA	MG-NA	5.15	2.18	2.06
24	B	612	CLA	C4B-NB	5.14	1.39	1.35
29	A	413	DGD	C4D-C5D	5.11	1.63	1.53
24	B	606	CLA	MG-NC	-5.11	1.94	2.06
24	c	502	CLA	MG-NC	-5.11	1.94	2.06
24	d	403	CLA	C4B-NB	4.98	1.39	1.35
24	C	513	CLA	C4D-ND	-4.95	1.30	1.37
24	d	405	CLA	MG-NC	-4.94	1.94	2.06
27	d	407	PL9	C3-C4	-4.93	1.41	1.49
24	c	505	CLA	C4D-ND	-4.93	1.30	1.37
24	C	503	CLA	C4D-ND	-4.87	1.31	1.37
24	B	603	CLA	C4D-ND	-4.87	1.31	1.37
24	C	509	CLA	MG-NA	4.83	2.17	2.06
24	b	607	CLA	C1D-ND	4.81	1.43	1.37
24	B	607	CLA	C1D-ND	4.80	1.43	1.37
24	b	609	CLA	C4B-NB	4.78	1.39	1.35
24	c	508	CLA	C4D-ND	-4.75	1.31	1.37
27	A	410	PL9	C3-C4	-4.70	1.41	1.49
24	B	608	CLA	C4B-NB	4.69	1.39	1.35
24	B	610	CLA	C1D-ND	4.66	1.43	1.37
26	c	515	BCR	C30-C25	-4.65	1.47	1.53
24	d	404	CLA	C4B-NB	4.62	1.39	1.35
24	b	611	CLA	C4D-ND	-4.62	1.31	1.37
24	C	509	CLA	C4D-ND	-4.59	1.31	1.37
24	b	612	CLA	C4B-NB	4.57	1.39	1.35
24	B	607	CLA	C4D-ND	-4.56	1.31	1.37
34	F	102	HEM	C3C-C2C	-4.46	1.34	1.40
26	B	619	BCR	C1-C6	-4.46	1.47	1.53
24	c	507	CLA	C4D-ND	-4.45	1.31	1.37
34	e	102	HEM	C3C-C2C	-4.45	1.34	1.40
24	a	405	CLA	C4D-ND	-4.44	1.31	1.37
24	B	604	CLA	MG-NA	4.44	2.16	2.06
24	B	605	CLA	C4D-ND	-4.44	1.31	1.37
24	B	605	CLA	C4B-NB	4.43	1.39	1.35
26	h	103	BCR	C30-C25	-4.38	1.47	1.53
24	b	613	CLA	C4D-ND	-4.36	1.31	1.37
24	b	613	CLA	C4B-NB	4.36	1.39	1.35
33	D	409	LHG	P-O6	4.35	1.76	1.59
24	B	611	CLA	C4D-ND	-4.34	1.31	1.37
24	B	602	CLA	MG-NA	4.34	2.16	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	502	CLA	MG-NA	4.34	2.16	2.06
24	b	611	CLA	C4B-NB	4.33	1.39	1.35
24	b	603	CLA	C4D-ND	-4.32	1.31	1.37
24	C	508	CLA	MG-NC	-4.31	1.96	2.06
24	a	405	CLA	C4B-NB	4.31	1.39	1.35
27	a	409	PL9	C6-C1	-4.27	1.40	1.48
24	B	602	CLA	C1D-ND	4.27	1.43	1.37
29	H	102	DGD	O5D-C1E	4.27	1.47	1.40
24	B	608	CLA	C4D-ND	-4.27	1.31	1.37
24	A	408	CLA	MG-ND	-4.26	1.97	2.05
24	d	403	CLA	C4D-ND	-4.26	1.31	1.37
24	C	503	CLA	MG-ND	4.24	2.14	2.05
24	B	609	CLA	C1D-ND	4.23	1.43	1.37
26	B	617	BCR	C1-C6	-4.23	1.48	1.53
24	b	616	CLA	MG-ND	-4.23	1.97	2.05
24	B	609	CLA	MG-ND	-4.21	1.97	2.05
24	D	403	CLA	MG-ND	-4.21	1.97	2.05
24	a	407	CLA	MG-NC	-4.20	1.96	2.06
24	B	607	CLA	C4B-NB	4.20	1.39	1.35
24	A	406	CLA	C1D-ND	4.19	1.42	1.37
24	c	504	CLA	MG-ND	-4.19	1.97	2.05
24	B	608	CLA	C3B-C2B	-4.17	1.34	1.40
24	c	502	CLA	MG-NA	4.15	2.16	2.06
24	D	404	CLA	C1D-ND	4.12	1.42	1.37
24	c	502	CLA	C4B-NB	4.11	1.38	1.35
24	B	605	CLA	CHC-C1C	4.10	1.45	1.35
24	A	406	CLA	C4B-NB	4.09	1.38	1.35
24	C	511	CLA	C1D-ND	4.08	1.42	1.37
24	c	513	CLA	MG-ND	-4.08	1.97	2.05
24	c	506	CLA	C1D-ND	4.08	1.42	1.37
24	B	616	CLA	C1D-ND	4.05	1.42	1.37
24	b	605	CLA	C4D-ND	-4.04	1.32	1.37
27	A	410	PL9	C7-C3	-4.03	1.47	1.51
26	B	618	BCR	C30-C25	-4.02	1.48	1.53
24	b	607	CLA	C1B-NB	4.02	1.38	1.35
24	B	605	CLA	C1D-ND	4.01	1.42	1.37
24	b	613	CLA	MG-NC	-4.01	1.96	2.06
24	C	512	CLA	C1D-ND	4.01	1.42	1.37
26	c	514	BCR	C1-C6	-4.01	1.48	1.53
24	A	405	CLA	C4D-ND	-3.97	1.32	1.37
24	c	503	CLA	C4D-ND	-3.96	1.32	1.37
24	c	501	CLA	C1D-ND	3.94	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	b	619	BCR	C30-C25	-3.93	1.48	1.53
24	C	510	CLA	C4D-ND	-3.92	1.32	1.37
24	D	402	CLA	C1D-ND	3.92	1.42	1.37
24	d	403	CLA	CHC-C1C	3.92	1.45	1.35
24	b	614	CLA	C4D-ND	-3.91	1.32	1.37
24	B	607	CLA	C3B-C2B	-3.91	1.34	1.40
24	B	604	CLA	C4D-ND	-3.90	1.32	1.37
24	d	404	CLA	C4D-ND	-3.90	1.32	1.37
24	a	405	CLA	C3B-C2B	-3.89	1.35	1.40
26	H	101	BCR	C30-C25	-3.88	1.48	1.53
26	d	406	BCR	C1-C6	-3.87	1.48	1.53
24	C	502	CLA	C1D-ND	3.85	1.42	1.37
29	C	518	DGD	O3G-C3G	-3.85	1.36	1.43
27	d	407	PL9	C7-C8	-3.83	1.45	1.50
24	c	508	CLA	CHC-C1C	3.82	1.44	1.35
24	c	505	CLA	CHC-C1C	3.80	1.44	1.35
24	b	609	CLA	CHC-C1C	3.80	1.44	1.35
28	a	410	SQD	O48-C23	3.80	1.44	1.33
24	c	505	CLA	C3B-C2B	-3.79	1.35	1.40
24	c	503	CLA	C1D-ND	3.78	1.42	1.37
24	C	514	CLA	C1D-ND	3.77	1.42	1.37
24	C	507	CLA	C1D-ND	3.77	1.42	1.37
24	B	610	CLA	MG-ND	-3.76	1.98	2.05
24	B	606	CLA	C4D-ND	-3.76	1.32	1.37
24	c	511	CLA	CHC-C1C	3.75	1.44	1.35
24	a	407	CLA	C4D-ND	-3.74	1.32	1.37
24	b	604	CLA	MG-NA	3.74	2.15	2.06
35	v	201	HEC	CBB-CAB	-3.73	1.35	1.49
24	D	403	CLA	C4B-NB	3.73	1.38	1.35
24	A	406	CLA	C4D-ND	-3.72	1.32	1.37
26	Y	101	BCR	C30-C25	-3.72	1.48	1.53
24	B	614	CLA	C4D-ND	-3.71	1.32	1.37
24	c	506	CLA	C3B-C2B	-3.70	1.35	1.40
26	Y	101	BCR	C1-C6	-3.68	1.48	1.53
24	h	101	CLA	C1D-ND	3.67	1.42	1.37
24	c	513	CLA	MG-NA	3.67	2.15	2.06
24	D	403	CLA	C1D-ND	3.65	1.42	1.37
26	a	408	BCR	C1-C6	-3.65	1.48	1.53
29	C	516	DGD	C4E-C3E	3.64	1.61	1.52
24	C	512	CLA	C1B-NB	3.64	1.38	1.35
35	V	201	HEC	CBC-CAC	-3.63	1.35	1.49
26	C	515	BCR	C30-C25	-3.63	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	K	101	BCR	C30-C25	-3.63	1.48	1.53
26	c	515	BCR	C1-C6	-3.62	1.48	1.53
24	b	604	CLA	C4D-ND	-3.62	1.32	1.37
24	c	509	CLA	C4D-ND	-3.62	1.32	1.37
24	C	506	CLA	C4D-ND	-3.61	1.32	1.37
24	c	502	CLA	C4D-ND	-3.61	1.32	1.37
28	A	412	SQD	O47-C7	3.61	1.44	1.34
24	b	616	CLA	C1D-ND	3.60	1.42	1.37
28	A	412	SQD	O48-C23	3.60	1.43	1.33
28	a	411	SQD	O48-C23	3.60	1.43	1.33
24	a	404	CLA	C1D-ND	3.59	1.42	1.37
29	c	517	DGD	O2G-C2G	-3.59	1.37	1.46
24	C	511	CLA	C4D-ND	-3.59	1.32	1.37
24	B	601	CLA	C1D-ND	3.58	1.42	1.37
32	c	522	LMG	O1-C1	3.58	1.46	1.40
33	D	408	LHG	O8-C6	-3.57	1.37	1.45
29	a	412	DGD	O2G-C1B	3.57	1.44	1.34
24	B	610	CLA	C3B-C2B	-3.57	1.35	1.40
24	b	617	CLA	C4D-ND	-3.57	1.32	1.37
24	a	404	CLA	MG-NC	3.56	2.14	2.06
32	K	102	LMG	O7-C8	-3.55	1.37	1.46
26	D	405	BCR	C30-C25	-3.54	1.48	1.53
24	B	608	CLA	CMD-C2D	-3.53	1.43	1.50
32	d	411	LMG	O7-C8	-3.53	1.37	1.46
24	B	610	CLA	CHC-C1C	3.53	1.44	1.35
24	C	506	CLA	C3B-C2B	-3.53	1.35	1.40
26	k	101	BCR	C1-C6	-3.51	1.48	1.53
24	b	615	CLA	C1D-ND	3.51	1.42	1.37
24	c	507	CLA	C3B-C2B	-3.50	1.35	1.40
27	A	410	PL9	C7-C8	-3.50	1.45	1.50
24	b	605	CLA	C1D-ND	3.50	1.42	1.37
26	b	618	BCR	C1-C6	-3.50	1.49	1.53
29	c	516	DGD	O2E-C2E	-3.49	1.34	1.43
32	M	101	LMG	C1-C2	3.49	1.62	1.52
24	D	402	CLA	C3B-C2B	-3.49	1.35	1.40
24	B	608	CLA	CHC-C1C	3.49	1.43	1.35
24	C	510	CLA	C1D-ND	3.49	1.42	1.37
24	C	514	CLA	MG-ND	3.49	2.12	2.05
24	c	509	CLA	C1D-ND	3.48	1.42	1.37
35	V	201	HEC	CBB-CAB	-3.47	1.36	1.49
24	c	506	CLA	C4D-ND	-3.47	1.32	1.37
35	v	201	HEC	CBC-CAC	-3.47	1.36	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	508	CLA	C1D-ND	3.47	1.42	1.37
24	C	511	CLA	MG-NC	3.46	2.14	2.06
24	b	611	CLA	C1D-ND	3.46	1.42	1.37
28	a	411	SQD	O47-C7	3.46	1.44	1.34
29	a	412	DGD	C1G-C2G	3.45	1.61	1.50
32	M	101	LMG	C9-C8	3.45	1.61	1.50
24	C	506	CLA	CHC-C1C	3.45	1.43	1.35
24	B	604	CLA	C1D-ND	3.45	1.42	1.37
24	D	403	CLA	C4D-ND	-3.45	1.33	1.37
24	C	507	CLA	C4D-ND	-3.43	1.33	1.37
26	b	619	BCR	C1-C6	-3.41	1.49	1.53
28	F	101	SQD	O48-C23	3.41	1.43	1.33
24	c	512	CLA	MG-NA	3.41	2.14	2.06
24	B	604	CLA	MG-ND	-3.40	1.99	2.05
24	a	407	CLA	C4B-CHC	-3.40	1.31	1.41
24	c	501	CLA	C4D-ND	-3.40	1.33	1.37
34	e	102	HEM	C3C-CAC	3.39	1.54	1.47
24	A	408	CLA	C1D-ND	3.38	1.41	1.37
28	B	622	SQD	O47-C7	3.38	1.43	1.34
24	a	407	CLA	C1D-ND	3.38	1.41	1.37
24	c	512	CLA	C1D-ND	3.38	1.41	1.37
24	c	511	CLA	C1D-ND	3.38	1.41	1.37
24	c	509	CLA	CHC-C1C	3.35	1.43	1.35
24	B	615	CLA	CMB-C2B	-3.34	1.44	1.51
24	b	609	CLA	C4D-ND	-3.33	1.33	1.37
28	b	601	SQD	O48-C23	3.33	1.43	1.33
24	B	615	CLA	C4D-ND	-3.33	1.33	1.37
24	b	603	CLA	C1D-ND	3.33	1.41	1.37
24	B	610	CLA	CMB-C2B	-3.32	1.44	1.51
24	B	611	CLA	CHC-C1C	3.32	1.43	1.35
24	b	604	CLA	CHC-C1C	3.32	1.43	1.35
24	C	507	CLA	CHC-C1C	3.31	1.43	1.35
29	C	517	DGD	C4D-C3D	3.31	1.60	1.52
26	A	409	BCR	C1-C6	-3.30	1.49	1.53
24	b	615	CLA	MG-ND	3.30	2.12	2.05
24	b	606	CLA	C4D-ND	-3.30	1.33	1.37
26	b	620	BCR	C1-C6	-3.29	1.49	1.53
24	d	404	CLA	MG-ND	3.29	2.12	2.05
24	A	408	CLA	C4D-ND	-3.29	1.33	1.37
24	b	614	CLA	MG-ND	-3.28	1.99	2.05
24	c	504	CLA	C4D-ND	-3.27	1.33	1.37
24	C	514	CLA	C4D-ND	-3.27	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	B	622	SQD	O48-C23	3.27	1.42	1.33
24	b	615	CLA	CHC-C1C	3.26	1.43	1.35
24	c	513	CLA	CHC-C1C	3.25	1.43	1.35
24	c	510	CLA	C1D-ND	3.25	1.41	1.37
24	h	101	CLA	CHC-C1C	3.25	1.43	1.35
24	A	405	CLA	MG-NC	-3.25	1.98	2.06
29	c	518	DGD	C4D-C5D	3.25	1.59	1.53
24	a	405	CLA	C1D-ND	3.25	1.41	1.37
24	b	606	CLA	C1D-ND	3.24	1.41	1.37
24	C	504	CLA	CHC-C1C	3.24	1.43	1.35
24	c	512	CLA	C4D-ND	-3.24	1.33	1.37
26	b	602	BCR	C30-C25	-3.23	1.49	1.53
26	K	101	BCR	C1-C6	-3.22	1.49	1.53
34	F	102	HEM	C3C-CAC	3.22	1.54	1.47
24	B	604	CLA	C3B-C2B	-3.21	1.35	1.40
29	H	102	DGD	C4D-C5D	3.21	1.59	1.53
24	c	509	CLA	MG-NA	-3.21	1.98	2.06
24	B	603	CLA	C1D-ND	3.21	1.41	1.37
24	C	503	CLA	MG-NC	3.20	2.13	2.06
32	c	522	LMG	C4-C5	3.20	1.59	1.53
33	D	411	LHG	O7-C5	-3.20	1.38	1.46
29	c	518	DGD	O1G-C1G	-3.20	1.37	1.45
24	B	606	CLA	CHC-C1C	3.20	1.43	1.35
24	b	616	CLA	CHC-C1C	3.19	1.43	1.35
29	C	517	DGD	O2G-C2G	-3.19	1.38	1.46
24	b	616	CLA	CMB-C2B	-3.18	1.45	1.51
24	A	405	CLA	C1D-ND	3.18	1.41	1.37
24	D	403	CLA	MG-NC	3.18	2.13	2.06
24	b	608	CLA	CMD-C2D	-3.17	1.44	1.50
24	B	609	CLA	C3B-C2B	-3.17	1.36	1.40
24	B	601	CLA	MG-NC	-3.16	1.98	2.06
29	H	102	DGD	O1G-C1G	-3.16	1.37	1.45
24	a	407	CLA	CMB-C2B	-3.15	1.45	1.51
24	c	510	CLA	C4D-ND	-3.15	1.33	1.37
26	k	101	BCR	C30-C25	-3.14	1.49	1.53
32	D	410	LMG	C9-C8	3.14	1.60	1.50
24	D	402	CLA	CHC-C1C	3.14	1.43	1.35
24	a	405	CLA	CHC-C1C	3.14	1.43	1.35
32	D	407	LMG	C4-C3	3.13	1.60	1.52
25	a	406	PHO	CBD-CGD	-3.13	1.48	1.52
24	c	510	CLA	CHC-C1C	3.13	1.43	1.35
26	b	602	BCR	C1-C6	-3.13	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	f	101	SQD	O47-C7	3.12	1.43	1.34
24	C	507	CLA	C3B-C2B	-3.12	1.36	1.40
24	c	510	CLA	CMB-C2B	-3.11	1.45	1.51
24	b	608	CLA	C3B-C2B	-3.11	1.36	1.40
24	b	611	CLA	C3B-C2B	-3.11	1.36	1.40
26	B	618	BCR	C1-C6	-3.11	1.49	1.53
24	d	404	CLA	CHC-C1C	3.10	1.42	1.35
28	A	411	SQD	O47-C7	3.09	1.43	1.34
24	b	612	CLA	C3B-C2B	-3.09	1.36	1.40
29	c	517	DGD	O3D-C3D	-3.09	1.35	1.43
26	b	620	BCR	C30-C25	-3.09	1.49	1.53
24	B	602	CLA	CHC-C1C	3.08	1.42	1.35
26	B	617	BCR	C30-C25	-3.07	1.49	1.53
24	A	406	CLA	CMB-C2B	-3.06	1.45	1.51
24	B	616	CLA	CMB-C2B	-3.06	1.45	1.51
26	B	619	BCR	C30-C25	-3.06	1.49	1.53
28	b	601	SQD	O47-C7	3.05	1.42	1.34
26	t	101	BCR	C30-C25	-3.05	1.49	1.53
24	b	615	CLA	C4D-ND	-3.04	1.33	1.37
24	B	613	CLA	CHC-C1C	3.04	1.42	1.35
24	b	612	CLA	CMD-C2D	-3.04	1.44	1.50
24	B	616	CLA	C4D-ND	-3.03	1.33	1.37
24	D	404	CLA	CHC-C1C	3.02	1.42	1.35
24	B	615	CLA	MG-NA	3.02	2.13	2.06
24	c	511	CLA	MG-NC	3.02	2.13	2.06
24	B	605	CLA	MG-ND	-3.01	1.99	2.05
24	d	404	CLA	CMB-C2B	-3.01	1.45	1.51
24	C	511	CLA	CHC-C1C	3.00	1.42	1.35
29	a	412	DGD	O1G-C1A	3.00	1.42	1.33
24	c	511	CLA	C4D-ND	-3.00	1.33	1.37
24	b	604	CLA	C1D-ND	2.99	1.41	1.37
24	B	613	CLA	C4D-ND	-2.99	1.33	1.37
29	H	102	DGD	C3E-C2E	2.99	1.59	1.52
24	B	615	CLA	C3B-C2B	-2.99	1.36	1.40
24	b	617	CLA	C1D-ND	2.99	1.41	1.37
24	b	603	CLA	CHC-C1C	2.99	1.42	1.35
24	c	502	CLA	CHC-C1C	2.98	1.42	1.35
24	C	504	CLA	C1D-ND	2.98	1.41	1.37
24	C	513	CLA	CHC-C1C	2.98	1.42	1.35
24	b	606	CLA	CHC-C1C	2.97	1.42	1.35
24	B	614	CLA	C3B-C2B	-2.97	1.36	1.40
24	b	610	CLA	C1D-ND	2.96	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	612	CLA	CHC-C1C	2.96	1.42	1.35
24	b	617	CLA	MG-ND	-2.96	1.99	2.05
24	c	501	CLA	CHC-C1C	2.96	1.42	1.35
24	c	513	CLA	MG-NC	-2.96	1.99	2.06
29	c	516	DGD	O2G-C2G	-2.95	1.39	1.46
24	c	505	CLA	CMB-C2B	-2.95	1.45	1.51
27	d	407	PL9	C26-C24	-2.95	1.45	1.51
24	B	608	CLA	MG-ND	-2.95	1.99	2.05
24	C	504	CLA	C4D-ND	-2.95	1.33	1.37
29	c	517	DGD	O3G-C1D	-2.95	1.35	1.40
32	D	410	LMG	C7-C8	2.94	1.58	1.51
32	D	407	LMG	O2-C2	-2.94	1.36	1.43
24	b	617	CLA	CMB-C2B	-2.94	1.45	1.51
25	D	401	PHO	CAC-C3C	-2.93	1.47	1.52
24	b	615	CLA	MG-NC	2.93	2.13	2.06
32	c	519	LMG	C1-C2	2.92	1.60	1.52
24	B	614	CLA	CMB-C2B	-2.92	1.45	1.51
25	A	407	PHO	C3B-C2B	-2.91	1.36	1.40
24	C	505	CLA	C4D-ND	-2.91	1.33	1.37
24	d	404	CLA	MG-NA	2.91	2.13	2.06
24	C	512	CLA	CMB-C2B	-2.90	1.45	1.51
24	C	505	CLA	CMB-C2B	-2.90	1.45	1.51
24	B	602	CLA	CMB-C2B	-2.89	1.45	1.51
24	b	606	CLA	MG-NA	2.88	2.13	2.06
24	C	508	CLA	CHC-C1C	2.87	1.42	1.35
24	B	612	CLA	CHC-C1C	2.87	1.42	1.35
24	C	503	CLA	CHC-C1C	2.87	1.42	1.35
24	d	405	CLA	C3B-CAB	-2.87	1.42	1.47
28	f	101	SQD	O48-C23	2.87	1.41	1.33
24	c	513	CLA	C4D-ND	-2.87	1.33	1.37
24	b	617	CLA	C3B-C2B	-2.86	1.36	1.40
24	B	606	CLA	C1D-ND	2.86	1.41	1.37
24	C	509	CLA	CHC-C1C	2.86	1.42	1.35
24	c	502	CLA	C1D-ND	2.86	1.41	1.37
24	B	604	CLA	CHC-C1C	2.86	1.42	1.35
27	D	406	PL9	C41-C39	-2.85	1.45	1.51
24	B	607	CLA	CAC-C3C	-2.85	1.43	1.51
24	C	502	CLA	CHC-C1C	2.85	1.42	1.35
24	D	403	CLA	CMB-C2B	-2.85	1.45	1.51
24	C	508	CLA	C4D-ND	-2.84	1.33	1.37
24	b	613	CLA	CMC-C2C	-2.84	1.44	1.50
24	b	612	CLA	C4B-CHC	-2.84	1.33	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	506	CLA	C3B-CAB	-2.83	1.42	1.47
24	c	504	CLA	CHC-C1C	2.83	1.42	1.35
24	B	613	CLA	CMB-C2B	-2.83	1.45	1.51
24	b	617	CLA	C3B-CAB	-2.82	1.42	1.47
24	d	405	CLA	CHC-C1C	2.82	1.42	1.35
24	D	402	CLA	CMB-C2B	-2.82	1.45	1.51
24	B	615	CLA	C3B-CAB	-2.82	1.42	1.47
24	c	507	CLA	C3B-CAB	-2.81	1.42	1.47
24	C	502	CLA	CMD-C2D	-2.81	1.44	1.50
24	B	609	CLA	CMD-C2D	-2.81	1.44	1.50
33	l	101	LHG	O8-C23	2.81	1.41	1.33
24	B	602	CLA	MG-ND	-2.80	2.00	2.05
24	b	614	CLA	C1D-ND	2.80	1.41	1.37
24	C	502	CLA	CMB-C2B	-2.80	1.45	1.51
24	c	508	CLA	MG-NA	2.80	2.12	2.06
24	b	611	CLA	CHC-C1C	2.80	1.42	1.35
32	d	411	LMG	O6-C5	-2.79	1.37	1.44
24	A	405	CLA	MG-ND	-2.79	2.00	2.05
27	D	406	PL9	C7-C8	-2.79	1.46	1.50
24	B	608	CLA	C3B-CAB	-2.78	1.42	1.47
24	c	513	CLA	C1D-ND	2.78	1.41	1.37
24	b	611	CLA	C1C-NC	-2.78	1.33	1.37
24	D	404	CLA	CMB-C2B	-2.77	1.45	1.51
33	E	101	LHG	O8-C23	2.77	1.41	1.33
24	B	614	CLA	MG-NA	2.77	2.12	2.06
24	a	407	CLA	C3B-C2B	-2.77	1.36	1.40
33	D	408	LHG	O7-C5	-2.77	1.39	1.46
24	b	603	CLA	CMC-C2C	-2.76	1.44	1.50
24	D	404	CLA	CMD-C2D	-2.76	1.45	1.50
26	t	101	BCR	C1-C6	-2.76	1.50	1.53
32	b	623	LMG	O1-C7	-2.75	1.38	1.43
26	c	515	BCR	C33-C5	-2.75	1.46	1.50
29	C	518	DGD	O1G-C1G	-2.75	1.38	1.45
24	B	601	CLA	CHC-C1C	2.75	1.42	1.35
29	c	518	DGD	C2A-C1A	-2.75	1.42	1.50
24	C	511	CLA	MG-ND	-2.75	2.00	2.05
24	B	606	CLA	CMB-C2B	-2.74	1.45	1.51
24	a	407	CLA	CMD-C2D	-2.74	1.45	1.50
24	b	609	CLA	C3B-C2B	-2.73	1.36	1.40
24	b	607	CLA	C4D-ND	-2.73	1.33	1.37
24	b	613	CLA	CHC-C1C	2.73	1.42	1.35
32	K	102	LMG	C4-C3	2.73	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	615	CLA	CHC-C1C	2.73	1.42	1.35
24	c	505	CLA	C3B-CAB	-2.73	1.42	1.47
25	d	402	PHO	CHA-CBD	-2.73	1.49	1.52
29	C	517	DGD	O3D-C3D	-2.73	1.36	1.43
26	d	406	BCR	C30-C25	-2.72	1.50	1.53
24	b	605	CLA	CHC-C1C	2.72	1.41	1.35
24	d	403	CLA	CMD-C2D	-2.72	1.45	1.50
24	C	504	CLA	C3B-C2B	-2.72	1.36	1.40
24	C	507	CLA	MG-NA	2.72	2.12	2.06
24	b	607	CLA	CHC-C1C	2.72	1.41	1.35
24	c	508	CLA	CMB-C2B	-2.72	1.46	1.51
32	c	524	LMG	C4-C5	2.71	1.58	1.53
24	b	605	CLA	MG-ND	-2.71	2.00	2.05
24	c	508	CLA	C1D-ND	2.71	1.41	1.37
26	D	405	BCR	C1-C6	-2.70	1.50	1.53
24	a	404	CLA	MG-ND	2.70	2.11	2.05
29	A	413	DGD	C1E-C2E	2.70	1.60	1.52
24	h	101	CLA	C1B-NB	2.70	1.37	1.35
26	b	618	BCR	C30-C25	-2.70	1.50	1.53
24	c	501	CLA	CMB-C2B	-2.69	1.46	1.51
24	C	503	CLA	C1D-ND	2.69	1.41	1.37
24	a	404	CLA	CHC-C1C	2.69	1.41	1.35
24	C	514	CLA	CMB-C2B	-2.69	1.46	1.51
29	A	413	DGD	C4D-C3D	2.69	1.59	1.52
26	A	409	BCR	C33-C5	-2.69	1.46	1.50
24	A	408	CLA	CHC-C1C	2.68	1.41	1.35
24	c	507	CLA	MG-NC	-2.68	1.99	2.06
24	C	512	CLA	C4D-ND	-2.68	1.34	1.37
24	B	613	CLA	C1D-ND	2.68	1.41	1.37
24	d	405	CLA	O1D-CGD	2.67	1.27	1.21
27	d	407	PL9	C46-C44	-2.67	1.45	1.51
24	b	603	CLA	CMB-C2B	-2.67	1.46	1.51
28	A	411	SQD	O48-C23	2.67	1.41	1.33
24	c	503	CLA	CHC-C1C	2.66	1.41	1.35
24	b	615	CLA	CMC-C2C	-2.66	1.45	1.50
24	B	611	CLA	CMB-C2B	-2.66	1.46	1.51
24	A	406	CLA	C4B-CHC	-2.65	1.33	1.41
24	h	101	CLA	O2A-CGA	2.65	1.41	1.33
29	A	413	DGD	C3E-C2E	2.64	1.59	1.52
24	B	610	CLA	MG-NC	-2.64	2.00	2.06
24	C	511	CLA	CMB-C2B	-2.64	1.46	1.51
24	d	405	CLA	CMB-C2B	-2.63	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	610	CLA	C4D-ND	-2.63	1.34	1.37
24	B	606	CLA	C3B-C2B	-2.63	1.36	1.40
24	b	607	CLA	MG-ND	-2.63	2.00	2.05
24	B	601	CLA	C3B-C2B	-2.63	1.36	1.40
24	B	607	CLA	MG-NA	2.62	2.12	2.06
24	c	509	CLA	MG-NC	2.62	2.12	2.06
25	A	407	PHO	C1C-NC	-2.62	1.30	1.38
24	a	404	CLA	CMB-C2B	-2.62	1.46	1.51
24	b	617	CLA	CAA-C2A	-2.62	1.49	1.54
24	b	616	CLA	CMD-C2D	-2.62	1.45	1.50
24	B	614	CLA	CHC-C1C	2.61	1.41	1.35
24	b	608	CLA	CHC-C1C	2.61	1.41	1.35
28	a	410	SQD	O47-C7	2.61	1.41	1.34
24	b	617	CLA	MG-NA	2.61	2.12	2.06
24	b	612	CLA	C4D-ND	-2.61	1.34	1.37
24	B	616	CLA	CMC-C2C	-2.61	1.45	1.50
25	d	402	PHO	CAC-C3C	-2.61	1.47	1.52
24	B	615	CLA	C5-C3	-2.61	1.45	1.51
29	h	104	DGD	C4D-C5D	2.61	1.58	1.53
24	c	512	CLA	CHC-C1C	2.61	1.41	1.35
27	D	406	PL9	C52-C5	-2.61	1.45	1.50
24	b	611	CLA	CMB-C2B	-2.61	1.46	1.51
24	b	609	CLA	C1D-ND	2.61	1.41	1.37
25	d	402	PHO	CMC-C2C	-2.61	1.45	1.51
24	c	506	CLA	CAC-C3C	-2.60	1.44	1.51
24	B	610	CLA	CMC-C2C	-2.60	1.45	1.50
24	C	505	CLA	CHC-C1C	2.60	1.41	1.35
25	A	407	PHO	CMC-C2C	-2.60	1.45	1.51
25	a	406	PHO	O2D-CGD	2.60	1.39	1.33
27	a	409	PL9	C53-C6	-2.60	1.45	1.50
27	A	410	PL9	C6-C1	-2.59	1.44	1.48
29	c	517	DGD	C4E-C3E	2.59	1.58	1.52
24	b	603	CLA	CMD-C2D	-2.59	1.45	1.50
24	c	507	CLA	C1D-ND	2.59	1.41	1.37
29	H	102	DGD	O2G-C2G	-2.59	1.40	1.46
24	b	611	CLA	C3D-C4D	2.59	1.50	1.44
24	b	616	CLA	C4D-ND	-2.58	1.34	1.37
24	B	609	CLA	C3B-CAB	-2.58	1.42	1.47
26	C	519	BCR	C30-C25	-2.58	1.50	1.53
29	C	517	DGD	C1G-C2G	2.57	1.58	1.50
24	c	513	CLA	CMB-C2B	-2.57	1.46	1.51
24	b	603	CLA	CAC-C3C	-2.57	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	513	CLA	MG-NC	-2.57	2.00	2.06
24	C	509	CLA	CMD-C2D	-2.57	1.45	1.50
24	c	506	CLA	MG-NC	2.57	2.12	2.06
29	C	516	DGD	C3E-C2E	2.57	1.58	1.52
24	b	617	CLA	CMD-C2D	-2.57	1.45	1.50
32	M	101	LMG	O3-C3	-2.56	1.36	1.43
24	C	512	CLA	CHC-C1C	2.56	1.41	1.35
24	C	510	CLA	CHC-C1C	2.56	1.41	1.35
24	D	403	CLA	CMD-C2D	-2.56	1.45	1.50
24	c	506	CLA	CHC-C1C	2.56	1.41	1.35
24	D	403	CLA	C1C-NC	-2.55	1.34	1.37
29	C	516	DGD	O3G-C3G	-2.55	1.39	1.43
33	d	410	LHG	O8-C6	-2.55	1.39	1.45
24	D	402	CLA	C4B-CHC	-2.55	1.33	1.41
26	b	602	BCR	C27-C26	-2.55	1.46	1.51
24	B	613	CLA	MG-ND	-2.55	2.00	2.05
28	f	101	SQD	O3-C3	-2.55	1.37	1.43
24	b	614	CLA	CMB-C2B	-2.55	1.46	1.51
24	B	614	CLA	C3B-CAB	-2.54	1.42	1.47
24	B	614	CLA	C4B-CHC	-2.54	1.33	1.41
32	c	522	LMG	C7-C8	2.54	1.58	1.50
24	A	408	CLA	CMD-C2D	-2.53	1.45	1.50
29	c	517	DGD	C4D-C3D	2.53	1.58	1.52
24	h	101	CLA	C4D-ND	-2.53	1.34	1.37
29	h	104	DGD	C1E-C2E	2.52	1.59	1.52
24	B	606	CLA	C3B-CAB	-2.52	1.42	1.47
29	c	517	DGD	C4E-C5E	2.52	1.58	1.53
28	a	410	SQD	O3-C3	-2.52	1.37	1.43
24	c	508	CLA	MG-ND	2.52	2.10	2.05
24	A	408	CLA	CMB-C2B	-2.52	1.46	1.51
27	a	409	PL9	C25-C24	-2.52	1.44	1.50
34	e	102	HEM	CAB-C3B	2.51	1.54	1.47
24	b	610	CLA	C3B-CAB	-2.51	1.42	1.47
24	b	616	CLA	C3B-C2B	-2.51	1.36	1.40
24	C	504	CLA	CMB-C2B	-2.51	1.46	1.51
24	a	404	CLA	CMC-C2C	-2.51	1.45	1.50
24	A	406	CLA	MG-ND	-2.51	2.00	2.05
24	B	603	CLA	C3B-CAB	-2.50	1.42	1.47
24	a	407	CLA	CMC-C2C	-2.50	1.45	1.50
26	C	519	BCR	C1-C6	-2.50	1.50	1.53
25	A	407	PHO	CAC-C3C	-2.50	1.47	1.52
24	B	601	CLA	CMB-C2B	-2.50	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	610	CLA	C4D-ND	-2.50	1.34	1.37
24	b	610	CLA	CMD-C2D	-2.50	1.45	1.50
24	C	502	CLA	C3D-C4D	2.50	1.49	1.44
24	h	101	CLA	CMC-C2C	-2.49	1.45	1.50
24	c	507	CLA	CMB-C2B	-2.49	1.46	1.51
29	C	518	DGD	O2G-C2G	-2.49	1.40	1.46
26	B	617	BCR	C33-C5	-2.48	1.46	1.50
24	C	502	CLA	C4D-ND	-2.48	1.34	1.37
24	B	607	CLA	CMB-C2B	-2.48	1.46	1.51
24	D	403	CLA	MG-NA	-2.48	2.00	2.06
24	C	513	CLA	CMD-C2D	-2.48	1.45	1.50
28	A	411	SQD	O2-C2	-2.47	1.37	1.43
24	C	514	CLA	C4B-CHC	-2.47	1.34	1.41
32	c	522	LMG	C4-C3	2.47	1.58	1.52
24	b	609	CLA	CMB-C2B	-2.47	1.46	1.51
34	F	102	HEM	CAB-C3B	2.47	1.54	1.47
24	b	604	CLA	MG-ND	-2.46	2.00	2.05
24	B	616	CLA	C3B-C2B	-2.46	1.37	1.40
24	d	403	CLA	O1D-CGD	2.46	1.27	1.21
24	c	507	CLA	CMC-C2C	-2.46	1.45	1.50
24	B	603	CLA	C1A-CHA	-2.46	1.32	1.43
24	A	406	CLA	C3B-C2B	-2.45	1.37	1.40
24	b	614	CLA	CMC-C2C	-2.45	1.45	1.50
24	b	606	CLA	C4B-CHC	-2.44	1.34	1.41
32	b	623	LMG	O6-C1	2.44	1.48	1.41
24	c	505	CLA	MG-NA	-2.44	2.00	2.06
25	a	406	PHO	CMB-C2B	-2.43	1.45	1.51
24	D	402	CLA	CMC-C2C	-2.43	1.45	1.50
27	a	409	PL9	C46-C44	-2.43	1.46	1.51
32	K	102	LMG	C1-C2	2.43	1.59	1.52
28	f	101	SQD	O2-C2	-2.43	1.37	1.43
29	h	104	DGD	C3G-C2G	2.43	1.58	1.50
24	A	406	CLA	MG-NC	2.43	2.12	2.06
29	H	102	DGD	C4E-C5E	2.42	1.58	1.53
24	B	603	CLA	C3B-C2B	-2.42	1.37	1.40
24	B	612	CLA	CMB-C2B	-2.42	1.46	1.51
24	C	504	CLA	C3B-CAB	-2.41	1.43	1.47
32	D	410	LMG	O8-C28	2.40	1.40	1.33
24	C	506	CLA	CMB-C2B	-2.40	1.46	1.51
24	b	613	CLA	C1D-ND	2.40	1.40	1.37
24	b	614	CLA	C5-C3	-2.40	1.46	1.51
24	B	605	CLA	C3D-C4D	2.40	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	d	404	CLA	C1D-ND	2.40	1.40	1.37
24	b	616	CLA	C3B-CAB	-2.39	1.43	1.47
29	c	518	DGD	O2G-C1B	2.39	1.41	1.34
24	C	507	CLA	CMC-C2C	-2.39	1.45	1.50
24	C	512	CLA	C4B-CHC	-2.39	1.34	1.41
33	D	409	LHG	O3-C3	-2.38	1.35	1.44
24	d	405	CLA	C3B-C2B	-2.38	1.37	1.40
33	E	101	LHG	P-O6	2.38	1.68	1.59
33	D	408	LHG	C24-C23	2.38	1.57	1.50
24	a	407	CLA	C1C-NC	-2.38	1.34	1.37
25	a	406	PHO	C3B-CAB	-2.38	1.43	1.47
24	C	512	CLA	CMC-C2C	-2.38	1.45	1.50
26	c	514	BCR	C30-C25	-2.38	1.50	1.53
24	c	508	CLA	CMC-C2C	-2.38	1.45	1.50
26	a	408	BCR	C38-C26	-2.38	1.47	1.50
24	D	403	CLA	C4B-CHC	-2.37	1.34	1.41
24	B	609	CLA	CMC-C2C	-2.37	1.45	1.50
25	D	401	PHO	CMD-C2D	-2.37	1.45	1.51
24	c	502	CLA	CMD-C2D	-2.36	1.45	1.50
24	C	513	CLA	C3B-C2B	-2.36	1.37	1.40
26	b	618	BCR	C33-C5	-2.36	1.47	1.50
26	H	101	BCR	C1-C6	-2.35	1.50	1.53
24	b	609	CLA	C3B-CAB	-2.35	1.43	1.47
33	D	411	LHG	O8-C6	2.35	1.50	1.45
24	C	506	CLA	CMC-C2C	-2.35	1.45	1.50
29	H	102	DGD	O6E-C1E	2.35	1.47	1.41
25	D	401	PHO	CBD-CGD	-2.35	1.49	1.52
24	B	609	CLA	C4B-CHC	-2.35	1.34	1.41
29	C	518	DGD	C4D-C5D	2.35	1.58	1.53
24	B	610	CLA	C3D-C4D	2.34	1.49	1.44
24	h	101	CLA	CMB-C2B	-2.34	1.46	1.51
32	b	623	LMG	C7-C8	2.34	1.57	1.50
24	B	615	CLA	MG-NC	2.34	2.11	2.06
24	B	616	CLA	C3B-CAB	-2.34	1.43	1.47
24	C	511	CLA	CMD-C2D	-2.34	1.45	1.50
24	b	605	CLA	CMC-C2C	-2.34	1.45	1.50
24	b	606	CLA	CMD-C2D	-2.34	1.45	1.50
33	D	411	LHG	C24-C23	2.34	1.57	1.50
24	C	509	CLA	C1D-ND	2.34	1.40	1.37
24	c	503	CLA	C3B-CAB	-2.33	1.43	1.47
29	A	413	DGD	O2G-C1B	2.33	1.40	1.34
24	c	508	CLA	CMD-C2D	-2.33	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	502	CLA	MG-NC	-2.32	2.00	2.06
24	A	405	CLA	CHC-C1C	2.32	1.40	1.35
24	C	504	CLA	MG-NC	2.32	2.11	2.06
24	b	611	CLA	CMA-C3A	-2.31	1.48	1.53
24	c	507	CLA	CHC-C1C	2.31	1.40	1.35
24	b	608	CLA	CMB-C2B	-2.31	1.46	1.51
24	C	510	CLA	O2D-CGD	2.31	1.38	1.33
32	c	522	LMG	C1-C2	2.30	1.59	1.52
24	A	406	CLA	C3B-CAB	-2.30	1.43	1.47
24	C	514	CLA	CHC-C1C	2.30	1.40	1.35
24	B	607	CLA	C4B-CHC	-2.30	1.34	1.41
24	C	510	CLA	CMB-C2B	-2.30	1.46	1.51
24	c	501	CLA	MG-NC	-2.30	2.00	2.06
24	d	405	CLA	CMD-C2D	-2.30	1.45	1.50
24	A	408	CLA	CMC-C2C	-2.30	1.45	1.50
24	a	405	CLA	CMB-C2B	-2.30	1.46	1.51
29	c	517	DGD	C3E-C2E	2.30	1.58	1.52
24	B	608	CLA	C1D-ND	2.30	1.40	1.37
32	b	623	LMG	C3-C2	2.29	1.58	1.52
29	C	517	DGD	C4E-C3E	2.29	1.58	1.52
24	b	610	CLA	CHC-C1C	2.29	1.40	1.35
24	B	614	CLA	CMC-C2C	-2.29	1.45	1.50
24	D	403	CLA	C3B-C2B	-2.29	1.37	1.40
24	h	101	CLA	C3B-CAB	-2.29	1.43	1.47
24	C	506	CLA	C4B-CHC	-2.29	1.34	1.41
24	B	606	CLA	CMC-C2C	-2.29	1.46	1.50
25	d	402	PHO	CMA-C3A	-2.28	1.49	1.53
24	b	616	CLA	CMC-C2C	-2.28	1.46	1.50
24	c	511	CLA	C1B-NB	2.28	1.37	1.35
24	c	504	CLA	CMB-C2B	-2.28	1.46	1.51
24	b	614	CLA	C3B-C2B	-2.28	1.37	1.40
24	C	507	CLA	C3B-CAB	-2.28	1.43	1.47
32	C	501	LMG	C4-C3	2.28	1.58	1.52
29	c	516	DGD	O5D-C1E	-2.28	1.36	1.40
29	c	517	DGD	O5D-C1E	2.28	1.44	1.40
24	b	604	CLA	C3B-CAB	-2.28	1.43	1.47
24	B	613	CLA	C3B-C2B	-2.28	1.37	1.40
24	c	501	CLA	C4B-CHC	-2.27	1.34	1.41
24	a	405	CLA	C3B-CAB	-2.27	1.43	1.47
24	b	609	CLA	MG-ND	-2.27	2.01	2.05
24	c	504	CLA	C1D-ND	2.27	1.40	1.37
24	D	404	CLA	C3B-CAB	-2.27	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	504	CLA	CMD-C2D	-2.27	1.46	1.50
24	b	607	CLA	CAC-C3C	-2.27	1.45	1.51
24	A	408	CLA	C4B-CHC	-2.27	1.34	1.41
24	B	609	CLA	C4D-ND	-2.26	1.34	1.37
32	h	102	LMG	O7-C10	2.26	1.38	1.30
27	D	406	PL9	C5-C4	-2.26	1.39	1.47
24	C	513	CLA	CAA-C2A	-2.26	1.49	1.54
24	B	609	CLA	CHC-C1C	2.25	1.40	1.35
24	b	614	CLA	C4B-CHC	-2.25	1.34	1.41
24	b	606	CLA	CMB-C2B	-2.25	1.47	1.51
26	a	408	BCR	C27-C26	-2.25	1.46	1.51
27	D	406	PL9	C15-C14	-2.24	1.44	1.50
32	M	101	LMG	O8-C28	2.24	1.39	1.33
24	c	506	CLA	C3B-CAB	-2.24	1.43	1.47
24	B	616	CLA	CHC-C1C	2.24	1.40	1.35
24	a	404	CLA	O2D-CED	-2.24	1.40	1.45
24	d	403	CLA	C1D-C2D	2.24	1.49	1.45
25	A	407	PHO	CMD-C2D	-2.23	1.46	1.51
24	C	510	CLA	CMC-C2C	-2.23	1.46	1.50
24	b	605	CLA	CMD-C2D	-2.23	1.46	1.50
24	c	503	CLA	CMB-C2B	-2.23	1.47	1.51
24	C	508	CLA	CMB-C2B	-2.23	1.47	1.51
24	c	512	CLA	CMD-C2D	-2.23	1.46	1.50
29	H	102	DGD	C6E-C5E	2.23	1.59	1.51
25	D	401	PHO	C3B-C2B	-2.23	1.37	1.40
32	d	411	LMG	O1-C7	-2.22	1.39	1.43
28	A	411	SQD	O4-C4	-2.22	1.37	1.43
24	B	602	CLA	C4D-ND	-2.22	1.34	1.37
24	A	405	CLA	CMB-C2B	-2.22	1.47	1.51
24	b	615	CLA	CMB-C2B	-2.22	1.47	1.51
24	b	607	CLA	CMB-C2B	-2.22	1.47	1.51
24	B	614	CLA	C1A-CHA	-2.22	1.33	1.43
24	C	509	CLA	C1D-C2D	2.22	1.49	1.45
24	c	504	CLA	O2D-CGD	2.22	1.38	1.33
24	B	613	CLA	C3B-CAB	-2.22	1.43	1.47
24	C	510	CLA	C3B-CAB	-2.21	1.43	1.47
29	h	104	DGD	O2D-C2D	-2.21	1.37	1.43
24	c	510	CLA	C3B-C2B	-2.21	1.37	1.40
26	t	101	BCR	C27-C26	-2.20	1.46	1.51
24	a	404	CLA	C1D-C2D	2.20	1.49	1.45
24	b	617	CLA	CHC-C1C	2.20	1.40	1.35
28	a	410	SQD	O4-C4	-2.20	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	605	CLA	C3B-C2B	-2.20	1.37	1.40
26	c	515	BCR	C36-C18	-2.19	1.46	1.50
24	A	408	CLA	C1C-NC	-2.19	1.34	1.37
32	c	522	LMG	C3-C2	2.19	1.57	1.52
24	b	604	CLA	C1A-CHA	-2.19	1.34	1.43
32	D	407	LMG	C7-C8	2.19	1.57	1.50
24	C	513	CLA	MG-ND	-2.18	2.01	2.05
24	B	604	CLA	O2D-CGD	2.18	1.38	1.33
24	c	506	CLA	C4B-CHC	-2.18	1.34	1.41
32	c	519	LMG	C3-C2	2.18	1.57	1.52
24	C	504	CLA	C4B-CHC	-2.18	1.34	1.41
32	c	519	LMG	C7-C8	2.18	1.57	1.50
24	a	404	CLA	O2D-CGD	2.18	1.38	1.33
33	D	411	LHG	O6-C4	-2.18	1.36	1.44
29	C	517	DGD	O5D-C6D	-2.17	1.39	1.43
28	f	101	SQD	O4-C4	-2.17	1.37	1.43
24	B	603	CLA	CHC-C1C	2.17	1.40	1.35
24	b	608	CLA	CMC-C2C	-2.17	1.46	1.50
24	h	101	CLA	CMD-C2D	-2.17	1.46	1.50
27	D	406	PL9	C10-C9	-2.17	1.45	1.50
34	e	102	HEM	CAA-C2A	2.17	1.55	1.52
24	b	609	CLA	MG-NA	2.17	2.11	2.06
24	B	608	CLA	CMC-C2C	-2.17	1.46	1.50
24	c	501	CLA	CAC-C3C	-2.17	1.45	1.51
26	A	409	BCR	C30-C25	-2.16	1.50	1.53
26	c	521	BCR	C30-C25	-2.16	1.50	1.53
24	A	408	CLA	C3D-C4D	2.16	1.49	1.44
24	B	601	CLA	CMD-C2D	-2.16	1.46	1.50
32	M	101	LMG	O7-C10	2.16	1.40	1.34
24	b	611	CLA	C1A-CHA	-2.16	1.34	1.43
24	C	502	CLA	C1D-C2D	2.16	1.49	1.45
24	C	508	CLA	C3B-C2B	-2.16	1.37	1.40
29	C	516	DGD	C2B-C1B	-2.16	1.44	1.50
24	b	608	CLA	C4D-ND	-2.15	1.34	1.37
29	c	517	DGD	O2E-C2E	-2.15	1.37	1.43
24	D	404	CLA	C1B-NB	2.15	1.37	1.35
25	d	402	PHO	C3B-CAB	-2.15	1.43	1.47
24	A	406	CLA	CHC-C1C	2.14	1.40	1.35
29	A	413	DGD	C6E-C5E	2.14	1.59	1.51
24	D	403	CLA	C1A-CHA	-2.13	1.34	1.43
27	d	407	PL9	C6-C1	-2.13	1.44	1.48
24	d	404	CLA	C3B-C2B	-2.13	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	602	CLA	C4B-CHC	-2.13	1.35	1.41
28	A	412	SQD	O47-C45	-2.13	1.43	1.47
24	b	609	CLA	C3D-C4D	2.13	1.49	1.44
24	b	604	CLA	CMB-C2B	-2.13	1.47	1.51
32	b	623	LMG	O8-C28	2.13	1.39	1.33
24	B	611	CLA	MG-NC	-2.13	2.01	2.06
24	B	602	CLA	C1A-CHA	-2.13	1.34	1.43
24	c	505	CLA	MG-ND	2.12	2.10	2.05
33	D	408	LHG	O6-C4	-2.12	1.36	1.44
24	C	503	CLA	C3D-C4D	2.12	1.49	1.44
32	M	101	LMG	O1-C7	-2.12	1.39	1.43
34	F	102	HEM	C1A-CHA	-2.12	1.35	1.41
24	c	506	CLA	CMD-C2D	-2.12	1.46	1.50
29	C	516	DGD	C2A-C1A	-2.12	1.44	1.50
24	b	612	CLA	CMB-C2B	-2.12	1.47	1.51
24	B	616	CLA	CMD-C2D	-2.12	1.46	1.50
34	e	102	HEM	C3B-C2B	-2.12	1.33	1.37
28	a	410	SQD	O2-C2	-2.12	1.38	1.43
24	A	405	CLA	CMC-C2C	-2.12	1.46	1.50
24	C	505	CLA	C1D-ND	2.11	1.40	1.37
24	B	605	CLA	O2D-CED	-2.11	1.40	1.45
24	B	615	CLA	C1D-ND	2.11	1.40	1.37
24	D	402	CLA	CAC-C3C	-2.11	1.45	1.51
29	A	413	DGD	C3G-C2G	2.11	1.57	1.50
24	c	513	CLA	CMD-C2D	-2.11	1.46	1.50
26	k	101	BCR	C38-C26	-2.11	1.47	1.50
24	B	613	CLA	CMC-C2C	-2.11	1.46	1.50
32	B	621	LMG	O8-C28	2.10	1.37	1.30
29	h	104	DGD	C4E-C5E	2.10	1.57	1.53
24	c	512	CLA	C3C-C2C	2.10	1.41	1.36
25	a	406	PHO	CMD-C2D	-2.10	1.46	1.51
24	d	403	CLA	CMB-C2B	-2.10	1.47	1.51
24	b	603	CLA	C3B-C2B	-2.10	1.37	1.40
33	D	411	LHG	O7-C7	2.10	1.40	1.34
24	D	403	CLA	CMC-C2C	-2.10	1.46	1.50
29	C	516	DGD	O1G-C1A	2.10	1.39	1.33
24	b	617	CLA	MG-NC	-2.10	2.01	2.06
24	A	405	CLA	C5-C3	-2.09	1.46	1.51
24	C	513	CLA	C3B-CAB	-2.09	1.43	1.47
24	c	507	CLA	C4B-CHC	-2.09	1.35	1.41
24	B	613	CLA	CHD-C1D	-2.09	1.34	1.38
24	b	614	CLA	CMD-C2D	-2.09	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	605	CLA	CMC-C2C	-2.09	1.46	1.50
28	F	101	SQD	O4-C4	-2.09	1.38	1.43
24	b	612	CLA	C1D-C2D	2.09	1.49	1.45
24	A	405	CLA	O2D-CED	-2.09	1.40	1.45
35	v	201	HEC	C4B-C3B	2.08	1.46	1.43
24	b	609	CLA	C1B-NB	2.08	1.37	1.35
26	C	515	BCR	C33-C5	-2.08	1.47	1.50
24	c	511	CLA	CMB-C2B	-2.08	1.47	1.51
25	D	401	PHO	C3B-CAB	-2.08	1.43	1.47
35	v	201	HEC	CMD-C2D	2.08	1.56	1.51
24	C	503	CLA	CMB-C2B	-2.08	1.47	1.51
24	A	406	CLA	CMD-C2D	-2.08	1.46	1.50
25	d	402	PHO	CMD-C2D	-2.08	1.46	1.51
24	B	613	CLA	CMD-C2D	-2.08	1.46	1.50
26	c	521	BCR	C38-C26	-2.08	1.47	1.50
24	B	601	CLA	C3B-CAB	-2.08	1.43	1.47
24	C	513	CLA	C3D-C4D	2.08	1.48	1.44
24	D	404	CLA	C4D-ND	-2.08	1.34	1.37
24	b	605	CLA	CMB-C2B	-2.07	1.47	1.51
24	B	616	CLA	O2D-CED	-2.07	1.40	1.45
24	b	604	CLA	CMD-C2D	-2.07	1.46	1.50
24	c	504	CLA	CMC-C2C	-2.07	1.46	1.50
24	B	612	CLA	C1A-CHA	-2.07	1.34	1.43
24	C	506	CLA	O1D-CGD	2.06	1.26	1.21
35	v	201	HEC	CAA-C2A	2.06	1.55	1.52
24	d	403	CLA	C3B-C2B	-2.06	1.37	1.40
24	B	615	CLA	CAC-C3C	-2.06	1.45	1.51
24	c	502	CLA	O2D-CGD	2.06	1.38	1.33
33	D	411	LHG	P-O4	-2.06	1.45	1.55
24	b	612	CLA	C1D-ND	2.05	1.40	1.37
32	c	524	LMG	C4-C3	2.05	1.57	1.52
33	D	408	LHG	P-O3	2.05	1.67	1.59
24	B	608	CLA	C4B-CHC	-2.05	1.35	1.41
33	d	410	LHG	P-O6	2.05	1.67	1.59
24	C	512	CLA	C3B-C2B	-2.05	1.37	1.40
24	A	406	CLA	CMC-C2C	-2.05	1.46	1.50
33	L	101	LHG	O7-C5	-2.05	1.41	1.46
24	c	507	CLA	C3D-C4D	2.05	1.48	1.44
28	F	101	SQD	O2-C2	-2.04	1.38	1.43
24	a	405	CLA	CAC-C3C	-2.04	1.45	1.51
24	b	615	CLA	C5-C3	-2.04	1.47	1.51
24	b	604	CLA	MG-NC	-2.04	2.01	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	K	102	LMG	C7-C8	2.04	1.56	1.50
24	B	611	CLA	C3B-CAB	-2.03	1.43	1.47
24	B	608	CLA	CAC-C3C	-2.03	1.45	1.51
32	D	407	LMG	C6-C5	2.03	1.58	1.51
24	C	511	CLA	C3D-C4D	2.03	1.48	1.44
24	B	610	CLA	C3B-CAB	-2.03	1.43	1.47
24	a	405	CLA	CMD-C2D	-2.03	1.46	1.50
24	B	616	CLA	C4B-CHC	-2.02	1.35	1.41
26	C	515	BCR	C36-C18	-2.02	1.46	1.50
34	F	102	HEM	CMD-C2D	2.02	1.55	1.50
24	B	612	CLA	CMD-C2D	-2.02	1.46	1.50
24	c	501	CLA	CMC-C2C	-2.02	1.46	1.50
24	C	506	CLA	MG-NA	2.02	2.11	2.06
24	C	504	CLA	CMC-C2C	-2.02	1.46	1.50
32	D	407	LMG	O3-C3	-2.02	1.38	1.43
24	C	505	CLA	CMC-C2C	-2.02	1.46	1.50
24	b	605	CLA	C3D-C4D	2.02	1.48	1.44
29	H	102	DGD	C1E-C2E	2.01	1.58	1.52
24	c	512	CLA	C3D-C4D	2.01	1.48	1.44
24	c	504	CLA	C3D-C4D	2.01	1.48	1.44
24	B	603	CLA	CMC-C2C	-2.01	1.46	1.50
33	E	101	LHG	P-O3	2.01	1.67	1.59
24	C	512	CLA	C4D-CHA	2.01	1.45	1.38
24	C	504	CLA	C5-C3	-2.00	1.47	1.51
24	C	512	CLA	C3D-C4D	2.00	1.48	1.44

All (1337) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	A	411	SQD	O6-C1-C2	9.52	123.17	108.30
28	A	411	SQD	O7-S-C6	9.51	118.24	106.94
28	a	410	SQD	O6-C1-C2	9.15	122.59	108.30
24	b	607	CLA	C4A-NA-C1A	8.45	110.51	106.71
24	a	404	CLA	C4A-NA-C1A	8.42	110.49	106.71
24	C	512	CLA	C4A-NA-C1A	8.17	110.38	106.71
24	B	604	CLA	C4A-NA-C1A	8.04	110.32	106.71
24	B	613	CLA	C4A-NA-C1A	7.99	110.30	106.71
28	b	601	SQD	O6-C1-C2	7.98	120.75	108.30
24	B	601	CLA	C4A-NA-C1A	7.63	110.14	106.71
24	C	508	CLA	C4A-NA-C1A	7.33	110.00	106.71
24	C	511	CLA	C4A-NA-C1A	6.87	109.80	106.71
24	b	616	CLA	C4A-NA-C1A	6.82	109.77	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	504	CLA	C4A-NA-C1A	6.81	109.77	106.71
24	c	509	CLA	C4A-NA-C1A	6.77	109.75	106.71
28	F	101	SQD	O9-S-C6	6.64	114.83	106.94
24	c	507	CLA	C4A-NA-C1A	6.62	109.68	106.71
24	D	402	CLA	C4A-NA-C1A	6.38	109.57	106.71
24	b	615	CLA	C4A-NA-C1A	6.36	109.57	106.71
24	C	514	CLA	C4A-NA-C1A	6.29	109.53	106.71
24	d	405	CLA	CHD-C1D-ND	-6.21	118.75	124.45
24	b	605	CLA	C4A-NA-C1A	6.13	109.46	106.71
24	C	503	CLA	C4A-NA-C1A	6.06	109.43	106.71
24	c	504	CLA	C4A-NA-C1A	5.88	109.35	106.71
24	c	503	CLA	C4A-NA-C1A	5.80	109.31	106.71
24	B	615	CLA	C4A-NA-C1A	5.77	109.30	106.71
24	C	505	CLA	CMB-C2B-C1B	-5.77	119.60	128.46
24	c	501	CLA	O2D-CGD-O1D	-5.73	112.64	123.84
27	a	409	PL9	C7-C3-C4	5.65	121.47	116.88
24	B	607	CLA	C4A-NA-C1A	5.65	109.25	106.71
24	d	404	CLA	C4A-NA-C1A	5.65	109.25	106.71
24	b	613	CLA	CMB-C2B-C1B	-5.55	119.93	128.46
28	B	622	SQD	O7-S-C6	5.55	113.54	106.94
24	b	616	CLA	CMB-C2B-C1B	-5.55	119.94	128.46
24	c	501	CLA	CMB-C2B-C1B	-5.52	119.98	128.46
28	f	101	SQD	O9-S-C6	5.45	113.42	106.94
24	c	505	CLA	C4A-NA-C1A	5.41	109.14	106.71
29	H	102	DGD	O3G-C3G-C2G	-5.35	97.98	110.90
24	B	606	CLA	CHD-C1D-ND	-5.33	119.55	124.45
24	b	603	CLA	C4A-NA-C1A	5.30	109.09	106.71
24	B	610	CLA	O2D-CGD-O1D	-5.29	113.49	123.84
24	b	617	CLA	O2D-CGD-O1D	-5.24	113.59	123.84
24	b	614	CLA	CMB-C2B-C1B	-5.24	120.42	128.46
28	a	410	SQD	O8-S-C6	5.22	114.05	105.74
24	b	617	CLA	C4A-NA-C1A	5.20	109.05	106.71
24	b	613	CLA	CMB-C2B-C3B	5.20	134.40	124.68
24	b	608	CLA	C4A-NA-C1A	5.16	109.02	106.71
24	c	502	CLA	C4A-NA-C1A	5.14	109.02	106.71
24	B	616	CLA	C4A-NA-C1A	5.13	109.01	106.71
28	a	411	SQD	O47-C7-C8	5.13	122.55	111.50
24	b	615	CLA	CMB-C2B-C1B	-5.07	120.67	128.46
24	c	510	CLA	C4A-NA-C1A	5.00	108.95	106.71
24	c	501	CLA	C4A-NA-C1A	4.99	108.95	106.71
24	b	604	CLA	O2D-CGD-O1D	-4.94	114.17	123.84
28	a	410	SQD	O9-S-C6	4.94	112.81	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	405	CLA	C4A-NA-C1A	4.94	108.92	106.71
24	c	510	CLA	O2D-CGD-CBD	4.79	119.77	111.27
28	A	411	SQD	O9-S-O7	-4.78	97.40	113.95
24	d	403	CLA	C4A-NA-C1A	4.78	108.86	106.71
24	C	514	CLA	CMB-C2B-C1B	-4.77	121.14	128.46
24	b	615	CLA	CHD-C1D-ND	-4.74	120.10	124.45
28	f	101	SQD	O6-C1-C2	4.73	115.68	108.30
32	b	623	LMG	O1-C1-C2	-4.72	100.94	108.30
24	b	603	CLA	O2D-CGD-O1D	-4.70	114.64	123.84
29	A	413	DGD	O5D-C6D-C5D	-4.68	100.39	109.05
24	C	510	CLA	C4A-NA-C1A	4.67	108.80	106.71
24	C	509	CLA	C4A-NA-C1A	4.64	108.79	106.71
24	c	507	CLA	CHD-C1D-ND	-4.62	120.21	124.45
24	B	615	CLA	CMB-C2B-C1B	-4.61	121.38	128.46
27	d	407	PL9	C40-C39-C41	4.60	123.00	115.27
29	C	517	DGD	O3G-C3G-C2G	-4.59	99.82	110.90
24	B	610	CLA	C1B-CHB-C4A	-4.58	121.05	130.12
24	c	510	CLA	O2D-CGD-O1D	-4.53	114.98	123.84
24	C	509	CLA	CHD-C1D-ND	-4.48	120.33	124.45
24	c	511	CLA	C4A-NA-C1A	4.44	108.70	106.71
24	b	604	CLA	O2D-CGD-CBD	4.44	119.16	111.27
24	B	612	CLA	C4A-NA-C1A	4.44	108.70	106.71
28	A	412	SQD	O47-C7-C8	4.43	121.05	111.50
25	d	402	PHO	O1D-CGD-CBD	4.42	132.10	124.74
24	C	509	CLA	O2D-CGD-O1D	-4.42	115.20	123.84
33	D	408	LHG	O4-P-O5	4.41	134.05	112.24
23	A	404	BCT	O2-C-O1	4.41	130.97	119.55
24	B	604	CLA	CMB-C2B-C1B	-4.37	121.75	128.46
26	K	101	BCR	C34-C9-C10	-4.35	116.83	122.92
24	c	504	CLA	CMB-C2B-C1B	-4.35	121.78	128.46
34	F	102	HEM	CBA-CAA-C2A	-4.34	105.22	112.62
24	B	609	CLA	CMB-C2B-C1B	-4.32	121.82	128.46
24	d	403	CLA	CHD-C1D-ND	-4.32	120.48	124.45
24	c	501	CLA	O2D-CGD-CBD	4.31	118.93	111.27
24	B	612	CLA	CMB-C2B-C1B	-4.30	121.86	128.46
24	c	512	CLA	C1-C2-C3	-4.30	118.61	126.04
24	c	513	CLA	C4A-NA-C1A	4.29	108.64	106.71
28	A	411	SQD	O9-S-C6	4.29	112.03	106.94
28	A	411	SQD	C1-C2-C3	-4.26	101.11	110.00
33	e	101	LHG	O4-P-O5	4.26	133.30	112.24
24	B	609	CLA	C4A-NA-C1A	4.25	108.62	106.71
24	b	615	CLA	CMB-C2B-C3B	4.23	132.60	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	502	CLA	CMB-C2B-C1B	-4.23	121.96	128.46
24	B	602	CLA	O2D-CGD-CBD	4.21	118.76	111.27
25	D	401	PHO	O1D-CGD-CBD	4.21	131.74	124.74
24	A	406	CLA	CMB-C2B-C1B	-4.20	122.01	128.46
24	c	506	CLA	C4A-NA-C1A	4.20	108.59	106.71
24	b	606	CLA	CMB-C2B-C1B	-4.19	122.02	128.46
24	B	611	CLA	O2D-CGD-CBD	4.19	118.72	111.27
33	D	409	LHG	O4-P-O5	4.18	132.92	112.24
24	C	507	CLA	CMB-C2B-C1B	-4.18	122.05	128.46
33	d	409	LHG	O4-P-O5	4.16	132.82	112.24
24	B	611	CLA	O2D-CGD-O1D	-4.16	115.70	123.84
24	B	605	CLA	CHD-C1D-ND	-4.15	120.64	124.45
24	b	603	CLA	CMB-C2B-C1B	-4.14	122.11	128.46
24	d	404	CLA	CMB-C2B-C1B	-4.13	122.11	128.46
28	B	622	SQD	C3-C4-C5	4.13	117.61	110.24
24	A	405	CLA	C4A-NA-C1A	4.13	108.56	106.71
24	b	611	CLA	CHD-C1D-ND	-4.11	120.67	124.45
29	A	413	DGD	C3G-C2G-C1G	-4.10	102.09	111.79
24	c	512	CLA	C4A-NA-C1A	4.09	108.55	106.71
24	b	617	CLA	O2D-CGD-CBD	4.09	118.53	111.27
24	B	601	CLA	O2D-CGD-O1D	-4.09	115.85	123.84
33	d	408	LHG	O4-P-O5	4.09	132.44	112.24
26	B	617	BCR	C2-C1-C6	4.08	116.77	110.48
28	b	601	SQD	O7-S-C6	4.08	111.78	106.94
24	d	403	CLA	CMB-C2B-C1B	-4.08	122.20	128.46
24	D	403	CLA	C1B-CHB-C4A	-4.07	122.05	130.12
24	b	604	CLA	C4-C3-C5	4.07	122.12	115.27
24	a	405	CLA	CHB-C4A-NA	4.06	130.13	124.51
33	d	410	LHG	O4-P-O5	4.06	132.31	112.24
28	B	622	SQD	O8-S-C6	4.04	112.19	105.74
24	B	611	CLA	CHD-C1D-ND	-4.03	120.75	124.45
24	C	502	CLA	O2D-CGD-O1D	-4.03	115.95	123.84
24	b	603	CLA	O2D-CGD-CBD	4.02	118.42	111.27
33	E	101	LHG	O4-P-O5	4.02	132.10	112.24
24	A	406	CLA	C4A-NA-C1A	4.02	108.51	106.71
24	A	408	CLA	O2D-CGD-O1D	-4.01	115.99	123.84
24	b	617	CLA	CMB-C2B-C1B	-4.01	122.30	128.46
24	c	510	CLA	CMB-C2B-C1B	-3.99	122.33	128.46
24	c	501	CLA	CMB-C2B-C3B	3.99	132.15	124.68
24	B	614	CLA	O2D-CGD-O1D	-3.99	116.03	123.84
24	C	502	CLA	C4A-NA-C1A	3.99	108.50	106.71
24	D	403	CLA	CMB-C2B-C1B	-3.98	122.34	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	504	CLA	C7-C6-C5	-3.98	102.54	113.36
24	b	607	CLA	O2D-CGD-O1D	-3.98	116.05	123.84
24	C	514	CLA	CMB-C2B-C3B	3.97	132.11	124.68
24	d	405	CLA	CMB-C2B-C1B	-3.97	122.36	128.46
24	C	503	CLA	CHD-C1D-ND	-3.97	120.81	124.45
28	B	622	SQD	O47-C7-C8	3.97	120.05	111.50
28	B	622	SQD	O6-C1-C2	3.96	114.48	108.30
29	C	518	DGD	O3G-C3G-C2G	-3.94	101.40	110.90
24	C	505	CLA	CMB-C2B-C3B	3.94	132.04	124.68
24	b	604	CLA	CMB-C2B-C1B	-3.93	122.42	128.46
27	d	407	PL9	C20-C19-C21	3.92	121.87	115.27
28	A	411	SQD	O47-C7-C8	3.92	119.94	111.50
24	B	616	CLA	CMB-C2B-C1B	-3.91	122.45	128.46
33	l	101	LHG	O4-P-O5	3.90	131.54	112.24
24	h	101	CLA	O2D-CGD-O1D	-3.90	116.21	123.84
24	d	404	CLA	CMB-C2B-C3B	3.90	131.97	124.68
24	a	405	CLA	CED-O2D-CGD	-3.88	107.16	115.94
33	D	411	LHG	O4-P-O5	3.88	131.41	112.24
24	b	609	CLA	CMB-C2B-C1B	-3.86	122.53	128.46
24	a	407	CLA	C1B-CHB-C4A	-3.86	122.48	130.12
24	B	610	CLA	C4A-NA-C1A	3.86	108.44	106.71
24	b	609	CLA	CMB-C2B-C3B	3.86	131.89	124.68
24	b	603	CLA	CHB-C4A-NA	3.85	129.83	124.51
24	A	406	CLA	CMB-C2B-C3B	3.85	131.87	124.68
24	b	606	CLA	C4-C3-C5	3.84	121.73	115.27
24	c	505	CLA	CHB-C4A-NA	3.84	129.82	124.51
24	b	611	CLA	O2D-CGD-O1D	-3.83	116.35	123.84
24	B	605	CLA	O1D-CGD-CBD	3.82	132.30	124.48
23	d	401	BCT	O2-C-O1	3.82	129.45	119.55
24	h	101	CLA	CMB-C2B-C1B	-3.78	122.66	128.46
34	e	102	HEM	CBD-CAD-C3D	-3.77	102.16	112.63
25	A	407	PHO	O2D-CGD-O1D	-3.77	116.47	123.84
24	b	612	CLA	CHD-C1D-ND	-3.76	121.00	124.45
24	C	503	CLA	O2D-CGD-O1D	-3.76	116.49	123.84
24	B	602	CLA	CHB-C4A-NA	3.75	129.70	124.51
24	C	504	CLA	O2A-C1-C2	-3.75	98.79	108.64
28	A	412	SQD	O47-C45-C44	3.75	116.49	107.93
24	B	616	CLA	O2D-CGD-O1D	-3.73	116.54	123.84
28	B	622	SQD	O9-S-O7	-3.73	101.03	113.95
33	D	411	LHG	O8-C23-O10	-3.73	114.18	123.59
24	C	502	CLA	O2D-CGD-CBD	3.73	117.89	111.27
24	B	606	CLA	C4A-NA-C1A	3.73	108.38	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	602	BCR	C38-C26-C27	-3.72	106.48	113.62
24	c	508	CLA	CMB-C2B-C1B	-3.71	122.76	128.46
24	C	507	CLA	CMB-C2B-C3B	3.71	131.61	124.68
24	c	502	CLA	CMB-C2B-C3B	3.71	131.61	124.68
24	b	615	CLA	O2D-CGD-O1D	-3.70	116.61	123.84
24	b	616	CLA	CMB-C2B-C3B	3.70	131.59	124.68
24	b	604	CLA	CHD-C1D-ND	-3.70	121.06	124.45
24	C	509	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
27	d	407	PL9	C7-C3-C4	3.69	119.88	116.88
24	C	512	CLA	CAC-C3C-C4C	3.69	129.60	124.81
24	b	613	CLA	CHD-C1D-ND	-3.68	121.07	124.45
24	C	508	CLA	CHD-C1D-ND	-3.68	121.07	124.45
24	b	609	CLA	C1B-CHB-C4A	-3.68	122.84	130.12
24	B	603	CLA	CMB-C2B-C3B	3.67	131.55	124.68
24	A	408	CLA	O2D-CGD-CBD	3.66	117.78	111.27
24	B	607	CLA	C2C-C1C-NC	3.66	113.40	109.97
24	b	614	CLA	CMB-C2B-C3B	3.66	131.52	124.68
24	C	503	CLA	CMB-C2B-C1B	-3.64	122.86	128.46
32	c	524	LMG	C1-O6-C5	-3.64	106.55	113.69
24	B	608	CLA	CMB-C2B-C1B	-3.64	122.88	128.46
24	a	407	CLA	O2D-CGD-O1D	-3.63	116.73	123.84
26	c	515	BCR	C27-C26-C25	3.63	128.00	122.73
24	b	608	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
24	B	605	CLA	C4A-NA-C1A	3.63	108.34	106.71
24	B	604	CLA	CHB-C4A-NA	3.62	129.52	124.51
24	c	507	CLA	CHB-C4A-NA	3.62	129.52	124.51
28	b	601	SQD	O8-S-C6	3.62	111.51	105.74
25	D	401	PHO	O2D-CGD-CBD	-3.62	106.41	111.00
24	d	405	CLA	CMB-C2B-C3B	3.62	131.45	124.68
24	C	502	CLA	CHD-C1D-ND	-3.61	121.13	124.45
24	C	509	CLA	CMB-C2B-C3B	3.61	131.43	124.68
33	L	101	LHG	O4-P-O5	3.61	130.07	112.24
25	D	401	PHO	CMB-C2B-C3B	3.61	131.43	124.68
24	A	408	CLA	C1D-ND-C4D	-3.60	103.78	106.33
26	b	619	BCR	C15-C14-C13	-3.60	122.17	127.31
33	d	409	LHG	O8-C23-C24	3.59	123.17	111.91
24	B	610	CLA	CHB-C4A-NA	3.58	129.47	124.51
26	B	619	BCR	C33-C5-C6	-3.58	120.51	124.53
24	b	610	CLA	CHD-C1D-ND	-3.57	121.18	124.45
29	C	516	DGD	O1G-C1A-C2A	-3.56	100.72	111.91
24	A	405	CLA	CHD-C1D-ND	-3.56	121.18	124.45
28	F	101	SQD	O8-S-C6	3.56	111.41	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	c	522	LMG	O6-C1-O1	-3.55	101.57	109.97
27	a	409	PL9	C7-C3-C2	-3.55	118.64	123.30
24	c	509	CLA	O2A-CGA-O1A	-3.55	114.64	123.59
24	B	612	CLA	CMB-C2B-C3B	3.54	131.30	124.68
24	B	603	CLA	CMB-C2B-C1B	-3.53	123.03	128.46
24	b	603	CLA	CMB-C2B-C3B	3.53	131.29	124.68
26	t	101	BCR	C15-C16-C17	-3.53	116.24	123.47
26	b	618	BCR	C15-C14-C13	-3.52	122.28	127.31
24	a	407	CLA	O2D-CGD-CBD	3.52	117.52	111.27
28	b	601	SQD	C1-C2-C3	-3.52	102.67	110.00
33	D	409	LHG	O8-C23-O10	-3.52	114.72	123.59
24	B	610	CLA	CHD-C1D-ND	-3.51	121.22	124.45
24	C	502	CLA	C1B-CHB-C4A	-3.51	123.17	130.12
24	B	613	CLA	C4-C3-C5	3.48	121.12	115.27
24	B	611	CLA	CMB-C2B-C1B	-3.48	123.12	128.46
24	b	608	CLA	C2D-C1D-ND	-3.48	107.54	110.10
24	c	509	CLA	O2D-CGD-O1D	-3.47	117.05	123.84
24	C	513	CLA	CHB-C4A-NA	3.47	129.31	124.51
28	B	622	SQD	C1-C2-C3	-3.47	102.77	110.00
28	b	601	SQD	O9-S-C6	3.47	111.06	106.94
24	A	408	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
26	c	515	BCR	C35-C13-C14	-3.47	118.06	122.92
25	d	402	PHO	CMC-C2C-C3C	3.46	131.47	124.94
24	a	404	CLA	C1B-CHB-C4A	-3.46	123.27	130.12
29	H	102	DGD	C1D-O6D-C5D	-3.45	106.91	113.69
24	h	101	CLA	C4A-NA-C1A	3.45	108.26	106.71
24	b	615	CLA	C1B-CHB-C4A	-3.45	123.29	130.12
24	B	605	CLA	C16-C15-C13	-3.45	104.78	115.92
24	b	612	CLA	O2D-CGD-CBD	3.44	117.39	111.27
28	A	411	SQD	C1-O5-C5	-3.44	106.93	113.69
24	b	611	CLA	CHB-C4A-NA	3.44	129.27	124.51
24	b	613	CLA	C1B-CHB-C4A	-3.44	123.31	130.12
24	c	509	CLA	CMB-C2B-C3B	3.43	131.09	124.68
24	d	403	CLA	CMB-C2B-C3B	3.42	131.08	124.68
26	b	620	BCR	C29-C30-C25	3.42	115.74	110.48
24	b	617	CLA	C1B-CHB-C4A	-3.42	123.35	130.12
26	C	519	BCR	C15-C16-C17	-3.42	116.47	123.47
24	C	506	CLA	CAC-C3C-C4C	3.41	129.24	124.81
28	B	622	SQD	O5-C5-C4	3.41	115.89	109.69
24	b	606	CLA	O2D-CGD-O1D	-3.41	117.17	123.84
24	B	605	CLA	CHB-C4A-NA	3.41	129.23	124.51
24	B	615	CLA	C1B-CHB-C4A	-3.41	123.37	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	604	CLA	CMB-C2B-C3B	3.40	131.04	124.68
24	b	610	CLA	O1D-CGD-CBD	3.40	131.43	124.48
24	c	503	CLA	CMB-C2B-C1B	-3.40	123.25	128.46
27	A	410	PL9	C7-C3-C4	3.39	119.63	116.88
24	b	606	CLA	C1-C2-C3	-3.39	120.18	126.04
24	b	617	CLA	CMB-C2B-C3B	3.39	131.01	124.68
24	b	609	CLA	CHB-C4A-NA	3.39	129.19	124.51
29	C	518	DGD	O3G-C1D-C2D	-3.38	103.02	108.30
28	b	601	SQD	C3-C4-C5	3.37	116.26	110.24
24	B	609	CLA	CMB-C2B-C3B	3.36	130.97	124.68
24	h	101	CLA	CHD-C1D-ND	-3.36	121.37	124.45
28	a	410	SQD	O8-S-O9	-3.36	103.08	111.27
24	B	603	CLA	O2A-CGA-O1A	-3.35	115.14	123.59
26	K	101	BCR	C11-C10-C9	-3.35	122.54	127.31
24	b	606	CLA	O1D-CGD-CBD	3.34	131.32	124.48
27	d	407	PL9	C22-C23-C24	-3.34	119.61	127.66
29	c	517	DGD	O3G-C1D-C2D	-3.34	103.09	108.30
28	b	601	SQD	O5-C5-C4	3.34	115.76	109.69
24	B	610	CLA	O2A-CGA-O1A	-3.34	115.16	123.59
29	c	516	DGD	O3G-C3G-C2G	-3.34	102.85	110.90
26	K	101	BCR	C33-C5-C6	-3.33	120.79	124.53
24	b	617	CLA	CHB-C4A-NA	3.33	129.11	124.51
24	C	512	CLA	CHB-C4A-NA	3.32	129.11	124.51
24	D	402	CLA	CHD-C1D-ND	-3.32	121.40	124.45
24	B	612	CLA	C11-C12-C13	-3.32	105.18	115.92
24	c	509	CLA	O1D-CGD-CBD	3.32	131.27	124.48
24	B	615	CLA	CMB-C2B-C3B	3.32	130.88	124.68
24	D	403	CLA	O2D-CGD-O1D	-3.31	117.36	123.84
24	c	511	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
28	f	101	SQD	O47-C7-C8	3.31	120.03	110.80
24	b	609	CLA	O2D-CGD-CBD	3.30	117.14	111.27
28	F	101	SQD	O9-S-O7	-3.30	102.51	113.95
24	c	504	CLA	CMB-C2B-C3B	3.30	130.85	124.68
24	C	509	CLA	C2D-C1D-ND	-3.29	107.68	110.10
26	B	619	BCR	C37-C22-C21	-3.28	118.32	122.92
24	C	510	CLA	CMB-C2B-C3B	3.28	130.82	124.68
24	B	604	CLA	CMB-C2B-C3B	3.28	130.82	124.68
24	b	606	CLA	C4A-NA-C1A	3.28	108.18	106.71
24	A	405	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
24	C	513	CLA	CMB-C2B-C3B	3.28	130.81	124.68
24	b	605	CLA	O2A-CGA-O1A	-3.28	115.33	123.59
29	c	518	DGD	O3G-C3G-C2G	-3.27	103.00	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	618	BCR	C33-C5-C6	-3.27	120.86	124.53
24	D	403	CLA	CMB-C2B-C3B	3.27	130.79	124.68
24	b	606	CLA	CHD-C1D-ND	-3.26	121.46	124.45
24	c	509	CLA	CHD-C1D-ND	-3.26	121.46	124.45
27	D	406	PL9	C37-C38-C39	-3.26	119.82	127.66
32	d	411	LMG	O2-C2-C1	-3.25	102.15	110.05
26	h	103	BCR	C30-C25-C26	-3.25	118.03	122.61
28	A	411	SQD	O47-C7-O49	-3.24	115.86	123.70
29	c	518	DGD	O6D-C1D-O3G	-3.24	102.30	109.97
24	c	502	CLA	C1B-CHB-C4A	-3.23	123.71	130.12
24	c	510	CLA	CHB-C4A-NA	3.23	128.98	124.51
26	c	521	BCR	C27-C26-C25	3.23	127.42	122.73
24	C	510	CLA	CMB-C2B-C1B	-3.23	123.50	128.46
24	d	405	CLA	C1B-CHB-C4A	-3.23	123.72	130.12
24	C	513	CLA	CHD-C1D-ND	-3.22	121.49	124.45
24	A	408	CLA	CED-O2D-CGD	-3.22	108.66	115.94
27	D	406	PL9	C22-C23-C24	-3.21	119.94	127.66
29	c	516	DGD	O3E-C3E-C2E	-3.20	102.94	110.35
29	A	413	DGD	C4E-C3E-C2E	-3.20	105.23	110.82
24	b	605	CLA	C1-C2-C3	-3.20	120.50	126.04
26	D	405	BCR	C2-C1-C6	3.20	115.41	110.48
24	B	614	CLA	C1B-CHB-C4A	-3.20	123.78	130.12
24	A	406	CLA	CED-O2D-CGD	-3.20	108.70	115.94
24	B	614	CLA	CHD-C1D-ND	-3.20	121.52	124.45
24	B	602	CLA	C4A-NA-C1A	3.19	108.14	106.71
32	C	501	LMG	O6-C1-O1	-3.19	102.42	109.97
24	B	606	CLA	CHD-C4C-NC	3.19	129.23	124.20
24	b	611	CLA	CMB-C2B-C3B	3.18	130.63	124.68
24	C	511	CLA	CMB-C2B-C1B	-3.18	123.57	128.46
24	c	507	CLA	C1B-CHB-C4A	-3.18	123.82	130.12
24	A	405	CLA	C1B-CHB-C4A	-3.18	123.82	130.12
24	B	605	CLA	O2D-CGD-O1D	-3.17	117.64	123.84
28	F	101	SQD	C3-C4-C5	3.16	115.88	110.24
26	c	514	BCR	C15-C16-C17	-3.16	117.00	123.47
24	c	503	CLA	C4-C3-C5	3.16	120.58	115.27
28	b	601	SQD	O9-S-O7	-3.15	103.06	113.95
26	b	602	BCR	C27-C26-C25	3.15	127.30	122.73
29	c	518	DGD	O3E-C3E-C2E	-3.14	103.08	110.35
24	c	504	CLA	O2D-CGD-CBD	3.14	116.85	111.27
24	C	514	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
32	D	407	LMG	C3-C4-C5	-3.14	104.64	110.24
24	c	512	CLA	O2D-CGD-O1D	-3.13	117.71	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	h	104	DGD	O3G-C3G-C2G	-3.13	103.34	110.90
24	B	616	CLA	C1-O2A-CGA	3.13	124.66	116.44
24	B	607	CLA	O2A-CGA-O1A	-3.13	115.69	123.59
29	c	517	DGD	O3G-C3G-C2G	-3.13	103.34	110.90
24	C	506	CLA	O1D-CGD-CBD	3.13	130.88	124.48
26	b	618	BCR	C2-C1-C6	3.13	115.29	110.48
24	b	605	CLA	CHB-C4A-NA	3.12	128.83	124.51
24	b	605	CLA	CHC-C1C-NC	3.12	128.93	124.20
24	C	503	CLA	CMB-C2B-C3B	3.11	130.50	124.68
24	a	405	CLA	O2D-CGD-O1D	-3.10	117.77	123.84
26	c	515	BCR	C33-C5-C6	-3.10	121.04	124.53
24	C	509	CLA	CHD-C1D-C2D	3.10	131.99	125.48
28	A	411	SQD	O2-C2-C1	3.10	117.58	110.05
24	b	606	CLA	CMB-C2B-C3B	3.10	130.47	124.68
26	b	619	BCR	C30-C25-C26	-3.10	118.25	122.61
24	C	509	CLA	C1D-ND-C4D	3.10	108.53	106.33
24	B	608	CLA	CMB-C2B-C3B	3.09	130.46	124.68
26	C	515	BCR	C35-C13-C14	-3.09	118.59	122.92
24	A	406	CLA	C1B-CHB-C4A	-3.09	124.00	130.12
24	h	101	CLA	CMB-C2B-C3B	3.09	130.46	124.68
24	c	503	CLA	CMB-C2B-C3B	3.09	130.45	124.68
24	b	612	CLA	C2D-C1D-ND	-3.09	107.83	110.10
26	C	515	BCR	C33-C5-C6	-3.08	121.07	124.53
29	C	518	DGD	O3E-C3E-C2E	-3.08	103.22	110.35
32	M	101	LMG	O1-C1-C2	-3.08	103.50	108.30
26	c	515	BCR	C15-C14-C13	-3.08	122.92	127.31
24	A	405	CLA	CHB-C4A-NA	3.07	128.76	124.51
24	b	614	CLA	C2C-C1C-NC	3.06	112.84	109.97
24	B	604	CLA	C1B-CHB-C4A	-3.06	124.05	130.12
24	b	603	CLA	CHC-C1C-NC	3.06	128.85	124.20
24	b	613	CLA	O1D-CGD-CBD	3.06	130.75	124.48
24	B	606	CLA	CMB-C2B-C1B	-3.06	123.76	128.46
24	D	404	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
24	D	403	CLA	O2D-CGD-CBD	3.06	116.71	111.27
24	B	602	CLA	CMB-C2B-C1B	-3.06	123.76	128.46
28	f	101	SQD	O8-S-C6	3.06	110.61	105.74
24	c	510	CLA	CAA-CBA-CGA	-3.06	104.32	113.25
32	c	519	LMG	O6-C1-O1	-3.06	102.74	109.97
24	c	503	CLA	C1B-CHB-C4A	-3.06	124.06	130.12
26	B	617	BCR	C15-C14-C13	-3.06	122.95	127.31
24	b	607	CLA	CMB-C2B-C1B	-3.05	123.77	128.46
26	c	514	BCR	C27-C26-C25	3.05	127.16	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	505	CLA	CHD-C1D-ND	-3.05	121.65	124.45
32	b	621	LMG	O7-C10-O9	-3.04	116.35	123.70
24	b	605	CLA	CMB-C2B-C1B	-3.04	123.79	128.46
26	b	619	BCR	C8-C7-C6	-3.04	118.67	127.20
33	D	411	LHG	O8-C23-C24	3.04	121.44	111.91
24	C	510	CLA	CHD-C1D-ND	-3.04	121.66	124.45
28	b	601	SQD	O48-C23-C24	3.04	121.44	111.91
24	c	512	CLA	CMB-C2B-C3B	3.03	130.35	124.68
24	D	402	CLA	C1B-CHB-C4A	-3.02	124.13	130.12
24	c	507	CLA	C4-C3-C5	3.02	120.36	115.27
28	a	410	SQD	C1-C2-C3	-3.02	103.70	110.00
24	b	616	CLA	C6-C5-C3	-3.01	105.56	113.45
24	C	505	CLA	C4A-NA-C1A	3.01	108.06	106.71
27	A	410	PL9	O1-C4-C3	-3.01	117.40	120.72
26	K	101	BCR	C38-C26-C25	-3.01	121.15	124.53
27	d	407	PL9	O1-C4-C3	-3.01	117.41	120.72
24	b	604	CLA	C1B-CHB-C4A	-3.00	124.17	130.12
27	d	407	PL9	C41-C39-C38	-3.00	115.05	121.12
33	e	101	LHG	O8-C23-O10	-3.00	116.03	123.59
24	B	605	CLA	C4-C3-C5	3.00	120.31	115.27
32	b	621	LMG	O1-C7-C8	-3.00	103.67	110.90
24	c	512	CLA	CMB-C2B-C1B	-3.00	123.86	128.46
24	B	601	CLA	O1D-CGD-CBD	2.99	130.61	124.48
24	B	616	CLA	CMB-C2B-C3B	2.99	130.28	124.68
24	d	403	CLA	C1D-ND-C4D	2.99	108.46	106.33
25	A	407	PHO	O2D-CGD-CBD	2.99	114.78	111.00
24	c	509	CLA	CMB-C2B-C1B	-2.99	123.88	128.46
24	b	610	CLA	C1B-CHB-C4A	-2.98	124.21	130.12
24	b	608	CLA	CMB-C2B-C3B	2.98	130.25	124.68
32	K	102	LMG	O1-C7-C8	-2.98	103.71	110.90
26	C	515	BCR	C27-C26-C25	2.98	127.06	122.73
26	B	619	BCR	C38-C26-C25	-2.98	121.18	124.53
28	a	410	SQD	O47-C7-C8	2.98	117.92	111.50
28	B	622	SQD	C1-O5-C5	-2.97	107.86	113.69
26	B	617	BCR	C15-C16-C17	-2.97	117.40	123.47
33	E	101	LHG	O8-C23-C24	2.97	121.22	111.91
24	c	501	CLA	CED-O2D-CGD	-2.96	109.24	115.94
24	a	404	CLA	CMB-C2B-C3B	2.96	130.22	124.68
26	B	618	BCR	C3-C4-C5	-2.96	108.79	114.08
26	k	101	BCR	C27-C26-C25	2.96	127.03	122.73
33	D	411	LHG	O3-P-O5	-2.96	97.50	109.07
24	b	611	CLA	CAA-C2A-C3A	-2.96	104.68	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	606	CLA	CHD-C4C-C3C	-2.96	120.49	124.84
32	d	411	LMG	O6-C1-O1	-2.95	102.99	109.97
24	h	101	CLA	CBA-CAA-C2A	2.95	122.56	113.86
24	C	502	CLA	C1D-ND-C4D	-2.94	104.24	106.33
28	b	601	SQD	C45-O47-C7	2.94	125.04	117.79
26	B	618	BCR	C27-C26-C25	2.94	127.00	122.73
32	M	101	LMG	C8-O7-C10	2.94	125.03	117.79
24	c	508	CLA	CMB-C2B-C3B	2.94	130.17	124.68
27	A	410	PL9	C22-C23-C24	-2.93	120.59	127.66
24	D	402	CLA	CHB-C4A-NA	2.93	128.57	124.51
29	A	413	DGD	C1D-C2D-C3D	-2.93	103.89	110.00
24	A	408	CLA	C1B-CHB-C4A	-2.93	124.31	130.12
29	C	517	DGD	O6D-C1D-O3G	-2.93	103.04	109.97
26	A	409	BCR	C29-C30-C25	2.93	114.98	110.48
29	c	517	DGD	O2E-C2E-C1E	-2.92	102.94	110.05
24	B	611	CLA	CHD-C4C-NC	2.92	128.81	124.20
26	H	101	BCR	C16-C15-C14	-2.92	117.50	123.47
27	a	409	PL9	C22-C23-C24	-2.92	120.63	127.66
32	c	522	LMG	O3-C3-C2	-2.92	103.60	110.35
26	b	619	BCR	C35-C13-C14	-2.92	118.84	122.92
26	h	103	BCR	C27-C26-C25	2.92	126.97	122.73
24	B	610	CLA	O2D-CGD-CBD	2.91	116.44	111.27
24	b	607	CLA	C1C-C2C-C3C	-2.91	103.89	106.96
29	c	516	DGD	O6D-C1D-O3G	-2.91	103.08	109.97
26	b	602	BCR	C7-C8-C9	-2.91	121.84	126.23
29	h	104	DGD	C4D-C3D-C2D	-2.91	105.75	110.82
24	B	608	CLA	C4A-NA-C1A	2.90	108.01	106.71
33	D	411	LHG	C11-C10-C9	-2.90	99.68	114.42
29	a	412	DGD	C2G-O2G-C1B	2.90	124.94	117.79
28	b	601	SQD	O2-C2-C1	2.90	117.10	110.05
24	b	609	CLA	CMA-C3A-C4A	-2.90	103.97	111.77
24	B	602	CLA	C11-C12-C13	-2.90	106.54	115.92
26	a	408	BCR	C38-C26-C27	-2.90	108.04	113.62
24	b	614	CLA	O1D-CGD-CBD	2.90	130.42	124.48
24	B	607	CLA	CMB-C2B-C1B	-2.90	124.01	128.46
27	d	407	PL9	C36-C34-C33	-2.90	115.25	121.12
27	A	410	PL9	C36-C34-C33	-2.90	115.25	121.12
24	D	402	CLA	O2D-CGD-CBD	2.90	116.42	111.27
24	c	502	CLA	CHD-C1D-ND	-2.90	121.79	124.45
24	b	614	CLA	C4A-NA-C1A	2.89	108.01	106.71
24	B	616	CLA	C1B-CHB-C4A	-2.89	124.39	130.12
24	a	407	CLA	O2A-CGA-O1A	-2.89	116.29	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	h	103	BCR	C15-C16-C17	-2.89	117.55	123.47
24	b	605	CLA	C7-C6-C5	-2.89	105.51	113.36
26	b	618	BCR	C15-C16-C17	-2.89	117.56	123.47
24	b	609	CLA	CHD-C1D-ND	-2.89	121.80	124.45
27	d	407	PL9	C42-C43-C44	-2.89	120.71	127.66
24	B	603	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
32	D	407	LMG	O6-C1-O1	-2.88	103.15	109.97
24	b	611	CLA	C1B-CHB-C4A	-2.88	124.41	130.12
24	b	603	CLA	CHD-C1D-ND	-2.88	121.81	124.45
24	C	504	CLA	CHD-C1D-ND	-2.88	121.81	124.45
24	C	507	CLA	CHB-C4A-NA	2.88	128.49	124.51
24	A	408	CLA	CMB-C2B-C3B	2.87	130.06	124.68
29	C	516	DGD	O5D-C6D-C5D	-2.87	103.73	109.05
24	B	607	CLA	C1B-CHB-C4A	-2.87	124.43	130.12
24	B	615	CLA	C4-C3-C5	-2.87	110.44	115.27
24	C	513	CLA	C1-C2-C3	-2.87	121.08	126.04
24	c	501	CLA	O2A-CGA-O1A	-2.87	116.34	123.59
24	d	404	CLA	O2A-CGA-O1A	-2.87	116.34	123.59
35	V	201	HEC	CMC-C2C-C1C	-2.87	124.05	128.46
25	D	401	PHO	C1-C2-C3	-2.86	121.09	126.04
24	c	506	CLA	CGD-CBD-CAD	-2.86	101.46	110.73
24	b	604	CLA	C5-C3-C2	-2.86	115.32	121.12
28	a	411	SQD	O48-C23-C24	2.86	120.89	111.91
24	C	507	CLA	C4A-NA-C1A	2.86	107.99	106.71
24	d	403	CLA	CHD-C1D-C2D	2.85	131.47	125.48
24	B	601	CLA	CMB-C2B-C1B	-2.85	124.08	128.46
24	C	510	CLA	CHB-C4A-NA	2.85	128.46	124.51
24	c	510	CLA	CMB-C2B-C3B	2.85	130.02	124.68
24	C	513	CLA	CMB-C2B-C1B	-2.85	124.08	128.46
24	B	602	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
32	d	411	LMG	C6-C5-C4	-2.85	106.33	113.00
34	F	102	HEM	CBD-CAD-C3D	-2.85	104.72	112.63
32	M	101	LMG	C40-C39-C38	-2.85	99.98	114.42
28	a	410	SQD	C1-O5-C5	-2.84	108.10	113.69
32	M	101	LMG	O1-C7-C8	-2.84	104.03	110.90
24	h	101	CLA	CHB-C4A-NA	2.84	128.44	124.51
24	B	614	CLA	O1D-CGD-CBD	2.84	130.30	124.48
27	D	406	PL9	C50-C49-C48	-2.84	114.44	122.65
24	c	512	CLA	CHB-C4A-NA	2.84	128.44	124.51
29	c	518	DGD	C3G-C2G-C1G	-2.84	105.08	111.79
24	b	614	CLA	CHA-C1A-NA	-2.83	119.91	126.40
24	C	511	CLA	CHB-C4A-NA	2.83	128.42	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	505	CLA	C7-C6-C5	-2.82	105.69	113.36
24	A	408	CLA	O2A-CGA-O1A	-2.82	116.46	123.59
24	B	614	CLA	C4-C3-C5	2.82	120.02	115.27
24	A	408	CLA	C4-C3-C5	2.82	120.02	115.27
28	F	101	SQD	C46-C45-C44	-2.82	104.33	113.70
25	d	402	PHO	CMB-C2B-C3B	2.82	129.94	124.68
29	h	104	DGD	C3D-C4D-C5D	-2.81	105.22	110.24
24	B	612	CLA	O2A-CGA-O1A	-2.81	116.49	123.59
24	c	508	CLA	CHB-C4A-NA	2.81	128.40	124.51
26	B	617	BCR	C35-C13-C14	-2.81	118.98	122.92
26	a	408	BCR	C33-C5-C6	-2.81	121.37	124.53
26	K	101	BCR	C2-C1-C6	2.81	114.81	110.48
26	a	408	BCR	C30-C25-C26	-2.81	118.66	122.61
26	B	619	BCR	C2-C1-C6	2.81	114.80	110.48
24	B	607	CLA	C1C-C2C-C3C	-2.81	104.01	106.96
24	B	608	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
29	C	517	DGD	O6E-C1E-O5D	-2.80	103.33	109.97
29	A	413	DGD	O6E-C1E-O5D	-2.80	103.34	109.97
34	e	102	HEM	CBA-CAA-C2A	-2.80	107.84	112.62
29	C	517	DGD	O5D-C6D-C5D	-2.80	103.87	109.05
26	k	101	BCR	C33-C5-C6	-2.80	121.39	124.53
24	h	101	CLA	C1B-CHB-C4A	-2.79	124.58	130.12
24	d	403	CLA	C2D-C1D-ND	-2.79	108.05	110.10
24	C	509	CLA	O2D-CGD-CBD	2.79	116.23	111.27
24	b	613	CLA	CHB-C4A-NA	2.79	128.37	124.51
24	c	504	CLA	O2A-CGA-O1A	-2.79	116.55	123.59
26	A	409	BCR	C27-C26-C25	2.79	126.78	122.73
26	K	101	BCR	C7-C8-C9	-2.79	122.03	126.23
26	B	618	BCR	C2-C1-C6	2.78	114.77	110.48
24	B	609	CLA	C1B-CHB-C4A	-2.78	124.62	130.12
24	C	502	CLA	CMB-C2B-C1B	-2.77	124.20	128.46
24	d	405	CLA	C1D-ND-C4D	-2.77	104.36	106.33
24	b	611	CLA	CMB-C2B-C1B	-2.77	124.21	128.46
24	C	513	CLA	C4A-NA-C1A	2.77	107.95	106.71
24	c	506	CLA	C4-C3-C5	2.77	119.92	115.27
32	M	101	LMG	O3-C3-C2	-2.77	103.96	110.35
24	b	611	CLA	CAA-CBA-CGA	-2.76	105.17	113.25
24	a	407	CLA	CMB-C2B-C1B	-2.76	124.22	128.46
24	c	503	CLA	C5-C3-C2	-2.76	115.53	121.12
24	b	616	CLA	C3B-C4B-NB	-2.76	105.64	109.21
24	c	505	CLA	O2A-CGA-O1A	-2.76	116.63	123.59
25	d	402	PHO	CMA-C3A-C4A	-2.76	108.34	114.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	d	410	LHG	O8-C6-C5	-2.75	100.42	108.43
24	b	604	CLA	O2A-CGA-O1A	-2.75	116.64	123.59
24	C	505	CLA	CHB-C4A-NA	2.75	128.32	124.51
24	C	511	CLA	O2A-CGA-O1A	-2.75	116.64	123.59
24	C	508	CLA	C1B-CHB-C4A	-2.75	124.67	130.12
27	D	406	PL9	C42-C43-C44	-2.75	121.04	127.66
24	a	404	CLA	CMB-C2B-C1B	-2.74	124.25	128.46
24	d	403	CLA	CHB-C4A-NA	2.74	128.31	124.51
24	C	511	CLA	CMB-C2B-C3B	2.74	129.81	124.68
29	H	102	DGD	CDB-CCB-CBB	-2.74	100.51	114.42
25	a	406	PHO	CMC-C2C-C3C	2.74	130.11	124.94
28	a	410	SQD	O10-C23-C24	-2.74	113.05	123.73
26	K	101	BCR	C34-C9-C8	-2.74	113.77	118.08
28	a	411	SQD	O48-C23-O10	-2.73	116.69	123.59
24	a	404	CLA	CHB-C4A-NA	2.73	128.29	124.51
26	h	103	BCR	C39-C30-C25	-2.73	105.87	110.30
24	d	405	CLA	C4D-CHA-C1A	2.73	124.57	121.25
32	C	501	LMG	O8-C28-O10	-2.73	116.70	123.59
32	D	407	LMG	O3-C3-C2	-2.73	104.04	110.35
29	c	517	DGD	O5D-C6D-C5D	-2.72	104.01	109.05
32	M	101	LMG	O6-C1-O1	-2.72	103.52	109.97
26	C	519	BCR	C29-C30-C25	2.72	114.67	110.48
28	B	622	SQD	O48-C23-C24	2.72	120.43	111.91
24	b	614	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
26	C	515	BCR	C15-C14-C13	-2.71	123.44	127.31
24	c	506	CLA	CHA-C1A-NA	-2.71	120.19	126.40
32	M	101	LMG	C9-C8-C7	-2.71	105.38	111.79
24	b	610	CLA	CHB-C4A-NA	2.71	128.26	124.51
24	B	605	CLA	C1-O2A-CGA	-2.70	109.35	116.44
35	v	201	HEC	CMB-C2B-C1B	-2.70	124.31	128.46
32	M	101	LMG	C37-C36-C35	-2.70	100.70	114.42
24	A	408	CLA	CHD-C1D-ND	-2.70	121.97	124.45
24	b	615	CLA	C1-C2-C3	-2.70	121.37	126.04
29	c	518	DGD	C3D-C4D-C5D	-2.70	105.42	110.24
24	C	514	CLA	CHD-C1D-ND	-2.70	121.97	124.45
28	F	101	SQD	O7-S-C6	-2.70	103.73	106.94
27	d	407	PL9	C37-C38-C39	-2.70	121.16	127.66
26	t	101	BCR	C24-C23-C22	-2.70	122.16	126.23
24	a	407	CLA	CHB-C4A-NA	2.70	128.24	124.51
24	B	610	CLA	O1D-CGD-CBD	2.70	130.00	124.48
24	b	612	CLA	CHD-C1D-C2D	2.70	131.13	125.48
24	B	601	CLA	CHD-C1D-ND	-2.70	121.98	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	513	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
24	B	611	CLA	CMB-C2B-C3B	2.69	129.71	124.68
24	C	503	CLA	O2D-CGD-CBD	2.69	116.05	111.27
24	A	405	CLA	O1D-CGD-CBD	2.69	129.99	124.48
29	C	518	DGD	CDB-CCB-CBB	-2.69	100.78	114.42
25	A	407	PHO	OBD-CAD-CBD	-2.69	121.88	125.82
24	C	505	CLA	O2A-CGA-O1A	-2.69	116.81	123.59
24	B	608	CLA	CHB-C4A-NA	2.69	128.23	124.51
24	d	403	CLA	C4D-CHA-C1A	2.68	124.52	121.25
24	c	507	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
32	c	524	LMG	O8-C28-O10	-2.68	116.83	123.59
26	B	618	BCR	C35-C13-C14	-2.67	119.18	122.92
24	B	616	CLA	O1D-CGD-CBD	2.67	129.95	124.48
26	B	619	BCR	C29-C30-C25	2.67	114.59	110.48
27	A	410	PL9	C20-C19-C21	2.67	119.76	115.27
29	a	412	DGD	O3G-C3G-C2G	-2.67	104.71	111.78
24	B	609	CLA	CHA-C1A-NA	-2.67	120.29	126.40
26	b	619	BCR	C11-C10-C9	-2.66	123.51	127.31
32	b	621	LMG	C40-C39-C38	-2.66	100.91	114.42
24	c	509	CLA	CHB-C4A-NA	2.66	128.19	124.51
32	b	621	LMG	O8-C28-O10	-2.66	116.89	123.59
24	B	607	CLA	CMB-C2B-C3B	2.65	129.64	124.68
24	C	513	CLA	C1B-CHB-C4A	-2.65	124.86	130.12
24	b	610	CLA	CMB-C2B-C3B	2.65	129.63	124.68
24	b	608	CLA	O1D-CGD-CBD	2.65	129.90	124.48
26	h	103	BCR	C35-C13-C12	2.65	122.25	118.08
26	B	617	BCR	C29-C30-C25	2.65	114.55	110.48
24	B	603	CLA	CHD-C4C-NC	2.64	128.37	124.20
26	h	103	BCR	C35-C13-C14	-2.64	119.22	122.92
29	C	516	DGD	C3D-C4D-C5D	-2.64	105.53	110.24
27	D	406	PL9	C12-C13-C14	-2.64	121.30	127.66
24	B	603	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
24	b	605	CLA	CMB-C2B-C3B	2.64	129.62	124.68
33	e	101	LHG	O8-C23-C24	2.64	120.18	111.91
34	F	102	HEM	C4C-CHD-C1D	2.64	126.04	122.56
24	C	504	CLA	C5-C3-C2	-2.64	115.78	121.12
26	K	101	BCR	C27-C26-C25	2.64	126.56	122.73
29	a	412	DGD	O1G-C1A-O1A	-2.63	116.94	123.59
24	B	614	CLA	CHB-C4A-NA	2.63	128.15	124.51
28	B	622	SQD	O47-C45-C46	2.63	117.92	108.40
29	c	517	DGD	C8B-C7B-C6B	-2.63	101.08	114.42
24	C	509	CLA	C3C-C4C-NC	-2.63	107.62	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	C	501	LMG	C38-C37-C36	-2.63	101.08	114.42
24	C	502	CLA	O2A-CGA-O1A	-2.63	116.96	123.59
26	C	519	BCR	C2-C1-C6	2.63	114.52	110.48
33	D	409	LHG	O8-C23-C24	2.62	120.13	111.91
32	D	407	LMG	O2-C2-C1	-2.62	103.69	110.05
24	a	407	CLA	C2C-C1C-NC	2.62	112.42	109.97
24	C	507	CLA	O2A-CGA-O1A	-2.62	116.99	123.59
26	B	619	BCR	C12-C13-C14	-2.62	114.93	118.94
24	b	606	CLA	O1A-CGA-CBA	2.61	133.93	123.73
28	A	411	SQD	O48-C23-O10	-2.61	116.99	123.59
32	c	524	LMG	O6-C1-O1	-2.61	103.79	109.97
24	B	603	CLA	CHD-C4C-C3C	-2.61	121.00	124.84
24	B	603	CLA	CHD-C1D-ND	-2.61	122.06	124.45
24	C	513	CLA	C7-C6-C5	-2.61	106.28	113.36
32	b	621	LMG	O6-C1-O1	-2.60	103.81	109.97
26	Y	101	BCR	C27-C26-C25	2.60	126.51	122.73
26	c	514	BCR	C33-C5-C6	-2.60	121.61	124.53
27	d	407	PL9	C40-C39-C38	-2.60	117.01	123.68
26	A	409	BCR	C29-C28-C27	2.60	117.18	111.38
28	a	410	SQD	O9-S-O7	-2.60	104.96	113.95
33	D	408	LHG	O8-C23-O10	-2.60	117.04	123.59
24	B	608	CLA	CAA-CBA-CGA	-2.59	105.67	113.25
33	d	410	LHG	C25-C24-C23	2.59	123.05	113.62
24	D	404	CLA	C1B-CHB-C4A	-2.59	124.99	130.12
26	b	620	BCR	C2-C1-C6	2.59	114.46	110.48
35	v	201	HEC	CMC-C2C-C1C	-2.59	124.49	128.46
24	B	610	CLA	C1D-ND-C4D	-2.58	104.50	106.33
33	D	409	LHG	O8-C6-C5	-2.58	100.92	108.43
34	e	102	HEM	CHC-C4B-C3B	2.58	128.52	124.57
24	B	607	CLA	O2A-C1-C2	-2.58	101.85	108.64
24	d	405	CLA	C4A-NA-C1A	2.58	107.86	106.71
24	d	404	CLA	CHD-C1D-ND	-2.58	122.09	124.45
26	a	408	BCR	C27-C26-C25	2.57	126.47	122.73
24	c	508	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
27	A	410	PL9	C27-C28-C29	-2.57	121.47	127.66
29	C	517	DGD	C1D-C2D-C3D	-2.57	104.65	110.00
26	H	101	BCR	C38-C26-C25	-2.57	121.64	124.53
24	b	610	CLA	CMB-C2B-C1B	-2.57	124.52	128.46
24	B	609	CLA	CED-O2D-CGD	2.57	121.74	115.94
27	D	406	PL9	C20-C19-C21	2.57	119.59	115.27
34	e	102	HEM	C3B-C2B-C1B	2.56	108.39	106.49
24	b	606	CLA	C4-C3-C2	-2.56	117.11	123.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	608	CLA	CHA-C1A-NA	-2.56	120.53	126.40
27	A	410	PL9	C30-C29-C28	-2.56	117.11	123.68
25	A	407	PHO	C1-O2A-CGA	2.56	123.16	116.44
24	c	503	CLA	C7-C6-C5	-2.56	106.41	113.36
24	h	101	CLA	O2D-CGD-CBD	2.56	115.81	111.27
24	a	407	CLA	CAA-CBA-CGA	-2.56	105.79	113.25
24	B	604	CLA	O2A-C1-C2	2.56	115.35	108.64
24	d	404	CLA	C6-C5-C3	2.55	120.15	113.45
24	d	404	CLA	C1B-CHB-C4A	-2.55	125.06	130.12
27	d	407	PL9	C50-C49-C48	-2.55	115.27	122.65
24	b	613	CLA	C11-C12-C13	-2.55	107.69	115.92
24	b	609	CLA	C11-C10-C8	-2.55	107.69	115.92
26	C	515	BCR	C15-C16-C17	-2.55	118.26	123.47
25	a	406	PHO	OBD-CAD-CBD	-2.54	122.09	125.82
29	H	102	DGD	C3G-C2G-C1G	-2.54	105.78	111.79
26	t	101	BCR	C38-C26-C27	-2.54	108.73	113.62
24	B	602	CLA	C2D-C1D-ND	-2.54	108.23	110.10
33	l	101	LHG	O8-C23-O10	-2.54	117.18	123.59
26	c	515	BCR	C15-C16-C17	-2.54	118.27	123.47
24	h	101	CLA	O2A-CGA-O1A	-2.54	117.19	123.59
26	H	101	BCR	C24-C23-C22	-2.53	122.41	126.23
26	B	618	BCR	C16-C15-C14	-2.53	118.28	123.47
33	d	408	LHG	C11-C10-C9	-2.53	101.56	114.42
27	a	409	PL9	C36-C34-C33	-2.53	116.00	121.12
27	D	406	PL9	C11-C9-C8	-2.53	116.00	121.12
24	b	616	CLA	CED-O2D-CGD	2.52	121.65	115.94
32	K	102	LMG	C38-C37-C36	-2.52	101.61	114.42
26	B	618	BCR	C11-C10-C9	-2.52	123.71	127.31
24	d	405	CLA	O1D-CGD-CBD	2.52	129.64	124.48
24	b	603	CLA	C2D-C1D-ND	-2.52	108.25	110.10
29	c	517	DGD	O2D-C2D-C1D	-2.52	103.92	110.05
24	C	514	CLA	CHB-C4A-NA	2.52	128.00	124.51
24	C	506	CLA	C4A-NA-C1A	2.52	107.84	106.71
24	B	605	CLA	C1B-CHB-C4A	-2.52	125.13	130.12
24	C	510	CLA	C1-C2-C3	-2.52	121.69	126.04
28	A	411	SQD	C3-C4-C5	2.51	114.72	110.24
26	H	101	BCR	C27-C26-C25	2.51	126.38	122.73
24	C	505	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
26	b	619	BCR	C33-C5-C6	-2.51	121.71	124.53
29	C	516	DGD	O6D-C1D-O3G	-2.51	104.03	109.97
29	c	516	DGD	C3G-C2G-C1G	-2.51	105.85	111.79
28	f	101	SQD	O9-S-O7	-2.51	105.27	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D	402	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
24	C	508	CLA	CAA-CBA-CGA	-2.51	105.93	113.25
26	b	618	BCR	C24-C23-C22	-2.51	122.45	126.23
24	B	606	CLA	CGD-CBD-CAD	-2.50	102.64	110.73
26	b	620	BCR	C38-C26-C25	-2.50	121.72	124.53
24	c	509	CLA	O2A-CGA-CBA	2.50	119.75	111.91
24	C	507	CLA	C1-C2-C3	-2.50	121.72	126.04
32	K	102	LMG	O2-C2-C1	-2.50	103.98	110.05
26	A	409	BCR	C2-C1-C6	2.50	114.33	110.48
29	c	516	DGD	CDB-CCB-CBB	-2.50	101.75	114.42
24	b	616	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
24	a	407	CLA	C4A-NA-C1A	2.50	107.83	106.71
26	C	515	BCR	C38-C26-C25	-2.50	121.73	124.53
29	H	102	DGD	C1D-C2D-C3D	-2.49	104.80	110.00
24	B	609	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
24	c	513	CLA	CHB-C4A-NA	2.49	127.95	124.51
24	a	405	CLA	O2D-CGD-CBD	2.49	115.69	111.27
24	c	513	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
29	h	104	DGD	O2D-C2D-C1D	-2.49	104.00	110.05
24	C	504	CLA	C4D-CHA-C1A	2.48	124.27	121.25
24	C	512	CLA	O2D-CGD-O1D	-2.48	118.98	123.84
29	C	517	DGD	O2D-C2D-C1D	-2.48	104.02	110.05
26	b	619	BCR	C27-C26-C25	2.48	126.33	122.73
24	C	514	CLA	O2A-CGA-O1A	-2.48	117.33	123.59
24	b	607	CLA	O2A-CGA-O1A	-2.48	117.33	123.59
24	B	611	CLA	C4A-NA-C1A	2.48	107.82	106.71
24	b	615	CLA	O2A-CGA-O1A	-2.48	117.34	123.59
24	B	615	CLA	CHB-C4A-NA	2.48	127.94	124.51
32	b	621	LMG	C9-C8-C7	-2.48	105.93	111.79
29	H	102	DGD	C1E-O6E-C5E	2.47	118.54	113.69
26	H	101	BCR	C29-C30-C25	2.47	114.29	110.48
24	B	609	CLA	C1D-CHD-C4C	-2.47	120.73	126.06
24	A	408	CLA	CHB-C4A-NA	2.47	127.93	124.51
26	b	619	BCR	C16-C15-C14	-2.47	118.42	123.47
24	B	613	CLA	CHD-C1D-ND	-2.47	122.19	124.45
24	C	506	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
24	B	604	CLA	C11-C12-C13	-2.47	107.95	115.92
24	c	504	CLA	CHB-C4A-NA	2.47	127.92	124.51
24	b	609	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
28	f	101	SQD	O48-C23-O10	-2.46	117.37	123.59
24	b	610	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
24	c	508	CLA	CHD-C1D-ND	-2.46	122.19	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	615	CLA	CMD-C2D-C1D	2.46	129.05	124.71
24	C	503	CLA	CAA-C2A-C3A	-2.46	106.04	112.78
33	l	101	LHG	O8-C23-C24	2.46	119.62	111.91
24	b	614	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
26	b	619	BCR	C35-C13-C12	2.46	121.95	118.08
26	d	406	BCR	C27-C26-C25	2.46	126.30	122.73
24	b	605	CLA	C4-C3-C5	2.46	119.40	115.27
24	c	505	CLA	C6-C7-C8	-2.45	107.98	115.92
24	c	506	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
28	a	411	SQD	O49-C7-C8	-2.45	114.17	123.73
26	B	619	BCR	C35-C13-C14	-2.45	119.49	122.92
24	c	506	CLA	C2A-C1A-CHA	2.45	128.15	123.86
24	b	612	CLA	C4A-NA-C1A	2.45	107.81	106.71
24	B	602	CLA	CHA-C1A-NA	-2.45	120.79	126.40
24	B	613	CLA	CAC-C3C-C4C	2.45	127.98	124.81
24	d	405	CLA	CHD-C1D-C2D	2.44	130.61	125.48
27	d	407	PL9	C45-C44-C46	-2.44	111.16	115.27
27	D	406	PL9	O1-C4-C3	-2.44	118.03	120.72
26	t	101	BCR	C19-C18-C17	-2.44	115.19	118.94
29	c	517	DGD	CDB-CCB-CBB	-2.44	102.03	114.42
33	d	408	LHG	O8-C6-C5	-2.44	101.33	108.43
27	d	407	PL9	C46-C47-C48	-2.44	103.86	111.88
29	C	518	DGD	O2D-C2D-C1D	-2.44	104.12	110.05
29	C	518	DGD	O6D-C1D-O3G	-2.44	104.20	109.97
24	b	607	CLA	C2C-C1C-NC	2.44	112.26	109.97
32	b	623	LMG	C1-O6-C5	-2.44	108.91	113.69
24	b	612	CLA	C2C-C1C-NC	2.43	112.25	109.97
26	c	514	BCR	C11-C10-C9	-2.43	123.84	127.31
24	B	601	CLA	CAA-C2A-C3A	-2.43	106.12	112.78
27	d	407	PL9	C7-C3-C2	-2.43	120.10	123.30
32	C	501	LMG	C1-O6-C5	-2.43	108.92	113.69
26	D	405	BCR	C16-C15-C14	-2.43	118.50	123.47
29	C	518	DGD	C3G-C2G-C1G	-2.43	106.05	111.79
26	C	519	BCR	C11-C10-C9	-2.43	123.85	127.31
29	C	517	DGD	O5D-C1E-C2E	2.43	112.09	108.30
27	d	407	PL9	C7-C8-C9	-2.43	122.75	126.79
24	C	505	CLA	CHD-C4C-C3C	-2.43	121.28	124.84
24	B	604	CLA	CHD-C1D-ND	-2.42	122.23	124.45
24	c	509	CLA	C3A-C2A-C1A	2.42	104.97	101.34
24	A	406	CLA	CAC-C3C-C4C	2.42	127.95	124.81
25	a	406	PHO	CMB-C2B-C3B	2.42	129.20	124.68
29	A	413	DGD	CDB-CCB-CBB	-2.42	102.15	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	511	CLA	CMB-C2B-C3B	2.42	129.20	124.68
24	b	615	CLA	O1D-CGD-CBD	2.42	129.43	124.48
29	C	518	DGD	O1G-C1A-C2A	-2.42	104.33	111.91
24	A	406	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
24	c	507	CLA	O2A-CGA-O1A	-2.41	117.50	123.59
32	c	522	LMG	O7-C10-O9	-2.41	117.87	123.70
24	b	614	CLA	CHB-C4A-NA	2.41	127.84	124.51
24	d	405	CLA	O2A-C1-C2	-2.41	102.30	108.64
26	c	514	BCR	C24-C23-C22	-2.41	122.59	126.23
26	c	515	BCR	C36-C18-C17	-2.41	119.55	122.92
25	A	407	PHO	O1D-CGD-CBD	2.41	128.75	124.74
29	c	516	DGD	CBB-CAB-C9B	-2.40	102.22	114.42
24	c	504	CLA	C7-C6-C5	-2.40	106.83	113.36
24	b	607	CLA	CMB-C2B-C3B	2.40	129.17	124.68
32	b	623	LMG	O2-C2-C1	-2.40	104.21	110.05
27	D	406	PL9	C7-C8-C9	-2.40	122.80	126.79
28	a	410	SQD	O7-S-C6	2.40	109.79	106.94
24	B	609	CLA	O2A-CGA-O1A	-2.40	117.54	123.59
24	h	101	CLA	C6-C5-C3	-2.40	107.17	113.45
24	b	610	CLA	C5-C3-C2	2.40	125.97	121.12
24	c	509	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
24	C	506	CLA	CMD-C2D-C1D	-2.40	120.49	124.71
24	C	503	CLA	O2A-CGA-O1A	-2.39	117.55	123.59
29	h	104	DGD	CDB-CCB-CBB	-2.39	102.28	114.42
32	c	522	LMG	C9-C8-C7	-2.39	106.14	111.79
24	C	514	CLA	C1-O2A-CGA	-2.39	110.18	116.44
24	C	513	CLA	CAA-CBA-CGA	-2.39	106.28	113.25
33	D	408	LHG	C11-C10-C9	-2.39	102.30	114.42
24	B	610	CLA	C11-C10-C8	-2.39	108.20	115.92
24	b	609	CLA	C6-C7-C8	-2.39	108.21	115.92
24	b	611	CLA	CHA-C1A-NA	-2.39	120.94	126.40
24	b	608	CLA	C1B-CHB-C4A	-2.38	125.39	130.12
24	B	612	CLA	C9-C8-C10	-2.38	102.66	111.29
28	F	101	SQD	C44-O6-C1	2.38	117.79	113.84
24	B	615	CLA	C4-C3-C2	2.38	129.79	123.68
29	C	516	DGD	CCB-CBB-CAB	-2.38	102.34	114.42
29	H	102	DGD	C8B-C7B-C6B	-2.38	102.36	114.42
29	h	104	DGD	O6D-C1D-O3G	-2.38	104.34	109.97
29	c	516	DGD	O6E-C5E-C4E	2.38	114.01	109.69
24	A	405	CLA	CMB-C2B-C3B	2.37	129.12	124.68
24	B	612	CLA	CHB-C4A-NA	2.37	127.80	124.51
24	h	101	CLA	O2A-C1-C2	2.37	114.87	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	511	CLA	CHA-C1A-NA	-2.37	120.97	126.40
24	B	603	CLA	C6-C5-C3	2.37	119.67	113.45
24	a	407	CLA	CMD-C2D-C3D	2.37	133.07	127.61
24	B	601	CLA	C2A-C1A-CHA	2.37	128.01	123.86
32	b	621	LMG	C38-C37-C36	-2.37	102.39	114.42
24	B	604	CLA	C1-C2-C3	2.37	130.14	126.04
24	c	505	CLA	O2D-CGD-CBD	2.37	115.48	111.27
26	B	619	BCR	C15-C16-C17	-2.37	118.62	123.47
27	d	407	PL9	C11-C9-C8	-2.37	116.33	121.12
24	b	606	CLA	C16-C15-C13	-2.37	108.27	115.92
24	b	613	CLA	CAC-C3C-C4C	2.37	127.88	124.81
33	d	408	LHG	O8-C23-C24	2.36	119.33	111.91
24	b	605	CLA	CHC-C1C-C2C	-2.36	120.18	126.72
24	b	614	CLA	CAC-C3C-C4C	2.36	127.88	124.81
25	d	402	PHO	C1-C2-C3	-2.36	121.96	126.04
29	C	517	DGD	CDB-CCB-CBB	-2.36	102.45	114.42
33	d	408	LHG	O8-C23-O10	-2.36	117.64	123.59
28	F	101	SQD	C4-C3-C2	2.36	114.94	110.82
24	b	604	CLA	C7-C6-C5	-2.36	106.96	113.36
24	B	609	CLA	O1D-CGD-CBD	2.36	129.30	124.48
24	D	402	CLA	CMB-C2B-C1B	-2.35	124.84	128.46
26	h	103	BCR	C3-C4-C5	-2.35	109.88	114.08
26	t	101	BCR	C11-C10-C9	-2.35	123.95	127.31
24	B	602	CLA	CHA-C4D-ND	2.35	137.42	132.50
26	c	515	BCR	C1-C6-C5	-2.35	119.30	122.61
24	d	405	CLA	CHA-C1A-NA	-2.35	121.02	126.40
24	h	101	CLA	C3B-C4B-NB	-2.35	106.17	109.21
24	B	602	CLA	CMB-C2B-C3B	2.35	129.07	124.68
27	A	410	PL9	C25-C24-C26	2.35	119.22	115.27
26	h	103	BCR	C7-C8-C9	-2.35	122.69	126.23
32	M	101	LMG	C35-C34-C33	-2.35	102.52	114.42
32	b	623	LMG	C8-O7-C10	2.34	123.56	117.79
26	Y	101	BCR	C39-C30-C25	-2.34	106.50	110.30
28	a	410	SQD	O48-C23-C24	2.34	119.26	111.91
29	c	518	DGD	O1G-C1A-C2A	-2.34	104.56	111.91
26	c	521	BCR	C24-C23-C22	-2.34	122.70	126.23
24	a	404	CLA	O2A-CGA-O1A	-2.34	117.69	123.59
24	d	403	CLA	CAC-C3C-C4C	2.34	127.84	124.81
24	C	511	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
24	C	503	CLA	C4D-CHA-C1A	2.34	124.09	121.25
24	B	611	CLA	C14-C13-C15	-2.34	102.83	111.29
24	B	610	CLA	CHD-C4C-NC	2.34	127.88	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	B	622	SQD	O10-C23-C24	-2.33	114.63	123.73
28	F	101	SQD	C1-O5-C5	-2.33	109.11	113.69
29	c	517	DGD	CBB-CAB-C9B	-2.33	102.58	114.42
26	b	620	BCR	C8-C7-C6	-2.33	120.66	127.20
28	A	412	SQD	O48-C23-C24	2.33	119.22	111.91
26	C	519	BCR	C37-C22-C21	-2.33	119.66	122.92
26	b	602	BCR	C33-C5-C6	-2.33	121.92	124.53
26	t	101	BCR	C7-C8-C9	-2.33	122.72	126.23
24	c	507	CLA	C5-C3-C2	-2.33	116.41	121.12
28	a	410	SQD	O5-C5-C4	2.33	113.92	109.69
24	B	606	CLA	C6-C5-C3	-2.32	107.36	113.45
24	B	611	CLA	CHD-C1D-C2D	2.32	130.36	125.48
24	B	613	CLA	CHA-C1A-NA	-2.32	121.08	126.40
24	d	405	CLA	C1-C2-C3	-2.32	122.03	126.04
26	b	618	BCR	C32-C1-C6	-2.32	106.53	110.30
29	a	412	DGD	O2G-C2G-C1G	2.32	116.80	108.40
26	b	619	BCR	C37-C22-C21	-2.32	119.67	122.92
26	c	515	BCR	C2-C1-C6	2.32	114.05	110.48
24	A	408	CLA	C4A-NA-C1A	2.32	107.75	106.71
33	l	101	LHG	O10-C23-C24	-2.32	114.70	123.73
32	b	621	LMG	O7-C10-C11	2.32	116.49	111.50
24	B	602	CLA	C4D-CHA-C1A	-2.32	118.43	121.25
24	B	611	CLA	C1B-CHB-C4A	-2.31	125.53	130.12
26	c	514	BCR	C15-C14-C13	-2.31	124.01	127.31
27	a	409	PL9	C11-C12-C13	-2.31	104.28	111.88
29	a	412	DGD	C1G-O1G-C1A	2.31	125.68	117.12
24	b	617	CLA	C4-C3-C5	2.31	119.15	115.27
24	B	615	CLA	C6-C7-C8	-2.31	108.46	115.92
24	c	505	CLA	CED-O2D-CGD	-2.31	110.72	115.94
24	B	613	CLA	C1D-ND-C4D	-2.31	104.70	106.33
24	B	604	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
24	C	513	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
34	e	102	HEM	CMC-C2C-C3C	2.30	128.99	124.68
27	a	409	PL9	C40-C39-C38	-2.30	117.77	123.68
29	A	413	DGD	O3G-C3G-C2G	-2.30	105.35	110.90
26	h	103	BCR	C15-C14-C13	-2.30	124.03	127.31
24	A	405	CLA	C3A-C2A-C1A	2.30	104.78	101.34
24	c	507	CLA	CHD-C4C-C3C	-2.30	121.46	124.84
26	c	521	BCR	C38-C26-C27	-2.30	109.20	113.62
24	B	606	CLA	CMB-C2B-C3B	2.30	128.97	124.68
24	B	613	CLA	C2A-C1A-CHA	2.29	127.87	123.86
29	C	518	DGD	CBB-CAB-C9B	-2.29	102.79	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	603	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
24	c	513	CLA	CMB-C2B-C1B	-2.29	124.94	128.46
32	b	623	LMG	C6-C5-C4	-2.29	107.64	113.00
32	h	102	LMG	O7-C10-O9	-2.29	117.59	123.30
24	B	611	CLA	O2A-CGA-O1A	-2.29	117.82	123.59
24	b	607	CLA	C4-C3-C5	2.29	119.12	115.27
24	A	406	CLA	CHD-C1D-ND	-2.29	122.35	124.45
24	b	614	CLA	C7-C6-C5	-2.29	107.15	113.36
25	d	402	PHO	O2D-CGD-O1D	-2.29	119.37	123.84
33	D	408	LHG	C20-C19-C18	-2.28	102.83	114.42
24	c	504	CLA	O2D-CGD-O1D	-2.28	119.38	123.84
32	C	501	LMG	C1-C2-C3	-2.28	105.24	110.00
24	A	406	CLA	CHB-C4A-NA	2.28	127.67	124.51
26	C	519	BCR	C15-C14-C13	-2.28	124.06	127.31
32	c	524	LMG	O5-C6-C5	-2.28	103.47	111.29
24	a	407	CLA	CMD-C2D-C1D	-2.28	120.69	124.71
29	a	412	DGD	C5B-C4B-C3B	-2.28	102.86	114.42
26	H	101	BCR	C16-C17-C18	-2.28	124.06	127.31
24	c	501	CLA	CHA-C1A-NA	-2.28	121.19	126.40
26	t	101	BCR	C36-C18-C19	2.28	121.66	118.08
24	B	613	CLA	C1-C2-C3	-2.27	122.11	126.04
24	c	507	CLA	O1D-CGD-CBD	2.27	129.14	124.48
29	A	413	DGD	C6D-O5D-C1E	2.27	118.17	113.74
29	a	412	DGD	CDB-CCB-CBB	-2.27	102.90	114.42
24	b	606	CLA	CHD-C4C-NC	2.27	127.78	124.20
26	d	406	BCR	C37-C22-C21	-2.27	119.75	122.92
24	b	604	CLA	C4A-NA-C1A	2.27	107.72	106.71
24	b	609	CLA	CHA-C1A-NA	-2.27	121.21	126.40
24	C	512	CLA	C4-C3-C5	2.26	119.08	115.27
26	K	101	BCR	C24-C23-C22	-2.26	122.81	126.23
24	b	606	CLA	CHA-C1A-NA	-2.26	121.22	126.40
27	A	410	PL9	C36-C37-C38	-2.26	104.45	111.88
33	D	411	LHG	C18-C17-C16	-2.26	102.95	114.42
25	A	407	PHO	C6-C7-C8	-2.26	108.61	115.92
24	a	404	CLA	CHD-C1D-ND	-2.26	122.38	124.45
27	D	406	PL9	C40-C39-C38	-2.26	117.89	123.68
24	B	613	CLA	CHB-C4A-NA	2.26	127.63	124.51
24	d	403	CLA	C1B-CHB-C4A	-2.25	125.65	130.12
29	C	518	DGD	C3G-O3G-C1D	-2.25	109.34	113.74
24	C	506	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
24	D	402	CLA	C16-C15-C13	-2.25	108.65	115.92
32	M	101	LMG	C1-O6-C5	-2.25	109.27	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	C	517	DGD	O3E-C3E-C2E	-2.25	105.15	110.35
24	c	502	CLA	CHB-C4A-NA	2.25	127.62	124.51
29	A	413	DGD	C5B-C4B-C3B	-2.25	103.01	114.42
26	b	618	BCR	C8-C7-C6	-2.25	120.89	127.20
24	C	510	CLA	CHA-C1A-NA	-2.25	121.25	126.40
24	b	604	CLA	CGD-CBD-CAD	-2.25	103.46	110.73
24	c	501	CLA	CHD-C1D-ND	-2.25	122.39	124.45
24	b	610	CLA	CHD-C4C-NC	2.25	127.74	124.20
24	b	605	CLA	C11-C10-C8	-2.25	108.66	115.92
26	h	103	BCR	C2-C1-C6	2.24	113.94	110.48
27	A	410	PL9	C40-C39-C38	-2.24	117.92	123.68
24	A	405	CLA	C4D-C3D-CAD	-2.24	105.45	108.10
24	b	610	CLA	C4A-NA-C1A	2.24	107.71	106.71
24	a	407	CLA	O2A-C1-C2	-2.24	102.75	108.64
24	c	507	CLA	CMB-C2B-C3B	2.24	128.86	124.68
24	c	511	CLA	O2D-CGD-O1D	-2.24	119.47	123.84
24	C	514	CLA	C4-C3-C5	2.24	119.03	115.27
29	h	104	DGD	CBB-CAB-C9B	-2.24	103.08	114.42
24	D	403	CLA	O2A-CGA-O1A	-2.23	117.95	123.59
32	M	101	LMG	C22-C21-C20	-2.23	103.08	114.42
24	c	512	CLA	O2A-CGA-O1A	-2.23	117.96	123.59
24	b	612	CLA	C11-C10-C8	-2.23	108.70	115.92
24	D	402	CLA	CMB-C2B-C3B	2.23	128.85	124.68
24	C	506	CLA	CMB-C2B-C1B	-2.23	125.04	128.46
29	C	516	DGD	C7B-C6B-C5B	-2.23	103.12	114.42
24	C	504	CLA	CHA-C1A-NA	-2.23	121.30	126.40
32	c	519	LMG	C40-C39-C38	-2.23	103.12	114.42
24	c	502	CLA	O2D-CGD-O1D	-2.22	119.49	123.84
24	c	507	CLA	CMB-C2B-C1B	-2.22	125.05	128.46
24	B	611	CLA	C2C-C1C-NC	2.22	112.06	109.97
26	a	408	BCR	C20-C21-C22	-2.22	124.14	127.31
24	C	512	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
32	M	101	LMG	O5-C6-C5	-2.22	103.67	111.29
33	d	409	LHG	O8-C23-O10	-2.22	117.98	123.59
29	C	516	DGD	CDB-CCB-CBB	-2.22	103.15	114.42
32	M	101	LMG	C38-C37-C36	-2.22	103.15	114.42
26	a	408	BCR	C24-C23-C22	-2.22	122.88	126.23
24	B	607	CLA	C4-C3-C5	2.22	119.00	115.27
29	h	104	DGD	C1E-O6E-C5E	2.22	118.04	113.69
24	B	611	CLA	CHB-C4A-NA	2.22	127.58	124.51
24	c	505	CLA	C1-C2-C3	-2.22	122.21	126.04
27	a	409	PL9	C45-C44-C46	-2.22	111.54	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	d	405	CLA	OBD-CAD-C3D	2.22	133.86	128.52
28	F	101	SQD	O6-C1-C2	2.22	111.77	108.30
24	B	616	CLA	CHB-C4A-NA	2.22	127.58	124.51
26	D	405	BCR	C24-C23-C22	-2.22	122.88	126.23
24	b	607	CLA	CHD-C1D-ND	-2.22	122.42	124.45
24	B	607	CLA	O1A-CGA-CBA	2.22	132.38	123.73
24	b	607	CLA	O2D-CGD-CBD	2.22	115.21	111.27
27	d	407	PL9	C8-C7-C3	2.21	118.24	111.98
29	c	517	DGD	C1D-C2D-C3D	-2.21	105.38	110.00
24	B	601	CLA	CHA-C4D-ND	2.21	137.13	132.50
24	C	506	CLA	C1B-CHB-C4A	-2.21	125.73	130.12
32	K	102	LMG	C3-C4-C5	-2.21	106.29	110.24
24	c	506	CLA	CED-O2D-CGD	2.21	120.94	115.94
24	B	605	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
24	C	514	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
24	D	403	CLA	CBA-CAA-C2A	-2.21	107.34	113.86
26	B	617	BCR	C33-C5-C6	-2.21	122.05	124.53
26	b	620	BCR	C16-C15-C14	-2.21	118.95	123.47
24	B	609	CLA	C7-C6-C5	-2.21	107.36	113.36
29	A	413	DGD	C4A-C3A-C2A	-2.21	105.25	113.19
26	b	619	BCR	C15-C16-C17	-2.21	118.95	123.47
24	D	403	CLA	C4A-NA-C1A	2.21	107.70	106.71
29	C	516	DGD	CAB-C9B-C8B	-2.20	103.24	114.42
26	c	514	BCR	C38-C26-C25	-2.20	122.05	124.53
28	b	601	SQD	O47-C7-C8	2.20	116.25	111.50
26	a	408	BCR	C11-C10-C9	-2.20	124.17	127.31
32	B	621	LMG	O7-C10-O9	-2.20	117.81	123.30
24	c	512	CLA	CHA-C1A-NA	-2.20	121.36	126.40
28	A	411	SQD	O3-C3-C4	2.20	115.43	110.35
24	B	603	CLA	CMD-C2D-C3D	2.20	132.67	127.61
24	d	404	CLA	O1D-CGD-CBD	2.19	128.97	124.48
26	t	101	BCR	C27-C26-C25	2.19	125.91	122.73
26	C	515	BCR	C35-C13-C12	2.19	121.53	118.08
24	b	613	CLA	C1-C2-C3	-2.19	122.25	126.04
24	b	603	CLA	CHC-C1C-C2C	-2.19	120.66	126.72
33	l	101	LHG	C11-C10-C9	-2.19	103.31	114.42
32	d	411	LMG	O1-C7-C8	-2.19	105.61	110.90
25	a	406	PHO	C5-C3-C2	2.19	125.55	121.12
26	b	618	BCR	C3-C4-C5	-2.19	110.17	114.08
25	a	406	PHO	C1-C2-C3	-2.19	122.26	126.04
24	c	508	CLA	C4A-NA-C1A	2.19	107.69	106.71
24	b	611	CLA	O1D-CGD-CBD	2.19	128.96	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	d	403	CLA	C11-C12-C13	-2.19	108.85	115.92
28	F	101	SQD	O5-C5-C4	2.19	113.67	109.69
24	C	508	CLA	CHB-C4A-NA	2.19	127.53	124.51
26	c	515	BCR	C30-C25-C26	-2.18	119.54	122.61
24	C	508	CLA	CGD-CBD-CAD	-2.18	103.67	110.73
26	c	521	BCR	C40-C30-C25	2.18	113.84	110.30
24	c	503	CLA	C11-C10-C8	-2.18	108.87	115.92
24	B	603	CLA	CHA-C1A-NA	-2.18	121.41	126.40
26	c	514	BCR	C34-C9-C10	-2.18	119.87	122.92
24	a	407	CLA	CMB-C2B-C3B	2.18	128.75	124.68
24	a	404	CLA	C11-C10-C8	-2.18	108.88	115.92
33	D	409	LHG	O3-P-O5	-2.18	100.56	109.07
32	C	501	LMG	C36-C35-C34	-2.18	103.38	114.42
29	C	516	DGD	C6B-C5B-C4B	-2.18	103.38	114.42
26	c	521	BCR	C16-C15-C14	-2.17	119.02	123.47
27	d	407	PL9	C31-C32-C33	-2.17	104.73	111.88
24	d	403	CLA	CHD-C4C-NC	2.17	127.63	124.20
24	B	603	CLA	C2C-C1C-NC	2.17	112.01	109.97
24	B	605	CLA	CMB-C2B-C3B	2.17	128.74	124.68
24	B	602	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
24	C	505	CLA	CHD-C4C-NC	2.17	127.63	124.20
26	a	408	BCR	C37-C22-C21	-2.17	119.88	122.92
24	a	405	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
34	e	102	HEM	CHB-C1B-NB	2.17	127.06	124.38
24	B	603	CLA	C4D-C3D-CAD	-2.17	105.54	108.10
26	b	620	BCR	C15-C16-C17	-2.17	119.03	123.47
26	Y	101	BCR	C33-C5-C6	-2.17	122.09	124.53
24	d	404	CLA	O2D-CGD-O1D	-2.17	119.60	123.84
26	h	103	BCR	C34-C9-C8	-2.17	114.66	118.08
24	c	504	CLA	C1D-ND-C4D	-2.17	104.80	106.33
32	d	411	LMG	C40-C39-C38	-2.17	103.43	114.42
26	b	620	BCR	C11-C10-C9	-2.17	124.22	127.31
33	D	409	LHG	C11-C10-C9	-2.17	103.43	114.42
27	A	410	PL9	C21-C19-C18	-2.16	116.74	121.12
24	b	616	CLA	C1-O2A-CGA	2.16	122.12	116.44
24	B	603	CLA	CHB-C4A-NA	2.16	127.50	124.51
32	K	102	LMG	O1-C1-C2	-2.16	104.92	108.30
32	B	621	LMG	C38-C37-C36	-2.16	103.44	114.42
24	B	616	CLA	CHA-C1A-NA	-2.16	121.44	126.40
26	C	515	BCR	C11-C10-C9	-2.16	124.23	127.31
32	c	519	LMG	C9-C8-C7	-2.16	106.68	111.79
26	B	619	BCR	C15-C14-C13	-2.16	124.23	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	407	PHO	CMC-C2C-C3C	2.16	129.01	124.94
27	d	407	PL9	C27-C28-C29	-2.15	122.47	127.66
24	d	405	CLA	C4-C3-C5	2.15	118.89	115.27
27	D	406	PL9	C11-C12-C13	-2.15	104.80	111.88
29	C	516	DGD	C8B-C7B-C6B	-2.15	103.50	114.42
24	B	605	CLA	C3A-C2A-C1A	2.15	104.56	101.34
32	C	501	LMG	O7-C10-O9	-2.15	118.50	123.70
28	A	411	SQD	O4-C4-C3	-2.15	105.38	110.35
24	c	502	CLA	C1-O2A-CGA	2.15	122.08	116.44
29	c	517	DGD	C7A-C6A-C5A	-2.15	103.52	114.42
24	C	503	CLA	CHA-C1A-NA	-2.15	121.48	126.40
24	c	512	CLA	CGD-CBD-CAD	2.15	117.69	110.73
26	Y	101	BCR	C23-C24-C25	-2.15	121.17	127.20
32	c	519	LMG	O7-C10-O9	-2.14	118.70	122.96
28	b	601	SQD	O47-C45-C46	2.14	116.17	108.40
24	C	504	CLA	C6-C5-C3	2.14	119.08	113.45
26	B	619	BCR	C32-C1-C6	-2.14	106.82	110.30
26	B	618	BCR	C8-C7-C6	-2.14	121.19	127.20
24	C	511	CLA	O2D-CGD-CBD	2.14	115.07	111.27
24	C	512	CLA	CHC-C1C-NC	2.14	127.45	124.20
24	c	513	CLA	C11-C12-C13	-2.14	109.00	115.92
24	b	608	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
24	B	608	CLA	CHD-C1D-ND	-2.14	122.49	124.45
26	h	103	BCR	C38-C26-C25	-2.14	122.12	124.53
26	H	101	BCR	C11-C10-C9	-2.14	124.26	127.31
26	c	521	BCR	C37-C22-C21	-2.14	119.93	122.92
29	H	102	DGD	CAB-C9B-C8B	-2.14	103.58	114.42
24	c	503	CLA	CHD-C1D-ND	-2.14	122.49	124.45
24	B	606	CLA	O1A-CGA-CBA	2.14	132.06	123.73
33	D	409	LHG	C27-C26-C25	-2.14	103.58	114.42
25	a	406	PHO	O2A-CGA-O1A	-2.13	118.21	123.59
27	a	409	PL9	C32-C33-C34	-2.13	122.53	127.66
24	B	612	CLA	C16-C15-C13	-2.13	109.03	115.92
26	c	515	BCR	C4-C5-C6	2.13	125.83	122.73
24	c	513	CLA	CMB-C2B-C3B	2.13	128.66	124.68
24	b	611	CLA	C11-C12-C13	-2.13	109.03	115.92
27	a	409	PL9	C12-C13-C14	-2.13	122.53	127.66
24	C	506	CLA	C11-C10-C8	-2.13	109.03	115.92
26	d	406	BCR	C38-C26-C25	-2.13	122.14	124.53
29	C	518	DGD	C5B-C4B-C3B	-2.13	103.62	114.42
24	b	607	CLA	CHA-C4D-ND	2.13	136.95	132.50
24	C	502	CLA	C3D-C4D-ND	2.13	113.68	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	K	101	BCR	C15-C16-C17	-2.13	119.12	123.47
24	C	505	CLA	C11-C10-C8	-2.13	109.05	115.92
24	A	408	CLA	C1D-CHD-C4C	-2.13	121.47	126.06
29	C	516	DGD	O2D-C2D-C1D	-2.12	104.88	110.05
33	l	101	LHG	C29-C28-C27	-2.12	103.64	114.42
24	D	403	CLA	CHB-C4A-NA	2.12	127.45	124.51
24	c	506	CLA	C1-C2-C3	-2.12	122.37	126.04
24	c	506	CLA	O1D-CGD-CBD	2.12	128.83	124.48
26	A	409	BCR	C8-C7-C6	-2.12	121.24	127.20
24	B	606	CLA	C1-C2-C3	-2.12	122.38	126.04
27	d	407	PL9	O2-C1-C2	-2.12	116.92	121.78
24	c	511	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
24	B	613	CLA	C1B-CHB-C4A	-2.12	125.92	130.12
35	v	201	HEC	CAD-CBD-CGD	-2.12	107.82	113.76
32	b	621	LMG	O1-C1-C2	-2.12	105.00	108.30
26	b	618	BCR	C35-C13-C14	-2.11	119.96	122.92
24	B	613	CLA	C11-C10-C8	-2.11	109.09	115.92
24	b	603	CLA	CHD-C1D-C2D	2.11	129.91	125.48
27	d	407	PL9	C31-C29-C28	2.11	125.39	121.12
24	c	507	CLA	CHD-C4C-NC	2.11	127.53	124.20
35	v	201	HEC	CBD-CAD-C3D	-2.11	109.02	112.62
24	c	506	CLA	CHB-C4A-NA	2.11	127.43	124.51
24	b	617	CLA	CMC-C2C-C1C	2.11	128.25	125.04
24	C	509	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
32	M	101	LMG	C31-C30-C29	-2.11	105.61	113.19
27	D	406	PL9	C35-C34-C36	2.11	118.81	115.27
24	b	606	CLA	C4D-CHA-C1A	2.11	123.81	121.25
32	c	522	LMG	C35-C34-C33	-2.11	103.74	114.42
24	a	407	CLA	C3B-C4B-NB	2.11	111.93	109.21
24	b	604	CLA	O2A-C1-C2	-2.10	103.10	108.64
24	b	605	CLA	CAC-C3C-C4C	2.10	127.54	124.81
24	b	612	CLA	CMB-C2B-C1B	-2.10	125.23	128.46
27	a	409	PL9	C27-C28-C29	-2.10	122.60	127.66
29	c	518	DGD	C1D-C2D-C3D	-2.10	105.62	110.00
26	c	515	BCR	C38-C26-C27	-2.10	109.58	113.62
24	B	615	CLA	CHD-C1D-ND	-2.10	122.52	124.45
24	c	513	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
26	d	406	BCR	C16-C15-C14	-2.10	119.17	123.47
26	C	519	BCR	C8-C7-C6	-2.10	121.31	127.20
27	D	406	PL9	C41-C39-C38	-2.10	116.87	121.12
26	h	103	BCR	C11-C10-C9	-2.10	124.31	127.31
33	d	409	LHG	C20-C19-C18	-2.10	103.77	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	504	CLA	C1-C2-C3	2.10	129.67	126.04
25	d	402	PHO	C1B-NB-C4B	2.10	111.40	107.09
29	C	518	DGD	C8B-C7B-C6B	-2.10	103.78	114.42
24	B	604	CLA	CED-O2D-CGD	2.09	120.67	115.94
24	B	601	CLA	CHA-C1A-NA	-2.09	121.60	126.40
28	B	622	SQD	C4-C3-C2	2.09	114.48	110.82
32	c	522	LMG	C42-C41-C40	-2.09	103.80	114.42
24	B	612	CLA	CHD-C4C-C3C	-2.09	121.77	124.84
24	C	509	CLA	CMC-C2C-C3C	2.09	131.79	126.12
24	B	616	CLA	CHA-C4D-ND	2.09	136.87	132.50
24	c	510	CLA	C1B-CHB-C4A	-2.09	125.98	130.12
24	A	406	CLA	C2C-C1C-NC	2.09	111.93	109.97
33	D	408	LHG	C27-C26-C25	-2.09	103.82	114.42
24	B	616	CLA	CAC-C3C-C4C	2.09	127.52	124.81
24	a	404	CLA	CAA-C2A-C1A	-2.09	105.14	111.97
29	c	518	DGD	O6E-C1E-O5D	-2.09	105.03	109.97
32	C	501	LMG	C40-C39-C38	-2.09	103.84	114.42
26	K	101	BCR	C35-C13-C14	-2.08	120.00	122.92
24	c	505	CLA	C11-C10-C8	-2.08	109.18	115.92
25	D	401	PHO	CBA-CAA-C2A	-2.08	107.72	113.81
24	b	612	CLA	C1-C2-C3	-2.08	122.44	126.04
27	A	410	PL9	C11-C9-C8	-2.08	116.91	121.12
24	a	404	CLA	C7-C6-C5	-2.08	107.71	113.36
26	d	406	BCR	C8-C7-C6	-2.08	121.36	127.20
26	A	409	BCR	C38-C26-C25	-2.08	122.19	124.53
24	b	611	CLA	CED-O2D-CGD	-2.08	111.24	115.94
26	b	618	BCR	C27-C26-C25	2.07	125.74	122.73
32	c	519	LMG	O8-C28-O10	-2.07	118.36	123.59
24	c	506	CLA	CMB-C2B-C3B	2.07	128.56	124.68
29	C	516	DGD	C9B-C8B-C7B	-2.07	103.90	114.42
24	c	511	CLA	O1A-CGA-CBA	2.07	131.82	123.73
24	b	607	CLA	CHD-C4C-NC	2.07	127.47	124.20
26	H	101	BCR	C35-C13-C12	2.07	121.34	118.08
24	b	614	CLA	C2A-C1A-CHA	2.07	127.48	123.86
24	b	609	CLA	C6-C5-C3	-2.07	108.03	113.45
24	C	504	CLA	O1D-CGD-CBD	2.07	128.72	124.48
28	A	411	SQD	O5-C1-C2	-2.07	105.97	110.35
32	b	623	LMG	C3-C4-C5	-2.07	106.55	110.24
33	D	411	LHG	C20-C19-C18	-2.07	103.94	114.42
29	c	516	DGD	C7A-C6A-C5A	-2.07	103.94	114.42
26	c	521	BCR	C30-C25-C26	-2.07	119.70	122.61
26	A	409	BCR	C15-C16-C17	-2.06	119.25	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	e	102	HEM	CMA-C3A-C4A	-2.06	125.29	128.46
35	V	201	HEC	CBD-CAD-C3D	-2.06	109.10	112.62
24	A	405	CLA	C7-C6-C5	-2.06	107.76	113.36
29	C	517	DGD	C5B-C4B-C3B	-2.06	103.97	114.42
27	D	406	PL9	C7-C3-C4	2.06	118.55	116.88
24	b	607	CLA	C2A-C1A-CHA	2.06	127.46	123.86
24	b	616	CLA	CHA-C4D-ND	2.06	136.80	132.50
29	C	518	DGD	O6D-C5D-C6D	-2.05	102.52	106.67
26	c	514	BCR	C10-C11-C12	-2.05	116.81	123.22
24	B	610	CLA	CMB-C2B-C1B	-2.05	125.31	128.46
24	b	607	CLA	CHA-C1A-NA	-2.05	121.70	126.40
26	B	619	BCR	C27-C26-C25	2.05	125.71	122.73
32	c	522	LMG	C33-C32-C31	-2.05	104.02	114.42
34	F	102	HEM	O2D-CGD-CBD	2.05	120.61	114.03
29	C	517	DGD	CAB-C9B-C8B	-2.05	104.03	114.42
24	b	611	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
24	a	405	CLA	C1B-CHB-C4A	-2.05	126.06	130.12
29	c	518	DGD	C9B-C8B-C7B	-2.05	104.03	114.42
24	C	512	CLA	O2D-CGD-CBD	2.04	114.90	111.27
25	d	402	PHO	C1A-C2A-C3A	-2.04	100.89	102.84
24	a	404	CLA	C1D-CHD-C4C	-2.04	121.65	126.06
27	a	409	PL9	O1-C4-C3	-2.04	118.47	120.72
24	b	609	CLA	C3B-C4B-NB	-2.04	106.57	109.21
26	C	519	BCR	C33-C5-C6	-2.04	122.23	124.53
24	A	406	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
26	K	101	BCR	C39-C30-C25	-2.04	106.99	110.30
24	b	604	CLA	C6-C5-C3	2.04	118.81	113.45
26	b	620	BCR	C7-C8-C9	-2.04	123.15	126.23
28	F	101	SQD	O48-C23-O10	-2.04	118.44	123.59
33	d	409	LHG	C29-C28-C27	-2.04	104.06	114.42
26	k	101	BCR	C1-C6-C5	-2.04	119.74	122.61
24	c	513	CLA	CHD-C1D-ND	-2.04	122.58	124.45
24	a	405	CLA	CHA-C1A-NA	-2.04	121.73	126.40
24	c	502	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
26	b	618	BCR	C29-C30-C25	2.04	113.62	110.48
24	C	506	CLA	CMD-C2D-C3D	2.04	132.30	127.61
24	C	507	CLA	CHA-C1A-NA	-2.04	121.73	126.40
29	C	517	DGD	C7B-C6B-C5B	-2.04	104.09	114.42
24	C	508	CLA	CHA-C4D-ND	2.04	136.76	132.50
24	c	505	CLA	O1A-CGA-CBA	2.04	131.67	123.73
24	c	507	CLA	O1A-CGA-CBA	2.03	131.67	123.73
32	C	501	LMG	O6-C1-C2	-2.03	106.04	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	d	406	BCR	C1-C6-C5	-2.03	119.75	122.61
24	c	506	CLA	O2A-C1-C2	-2.03	103.29	108.64
24	b	605	CLA	CMA-C3A-C4A	2.03	117.24	111.77
24	D	404	CLA	CHA-C1A-NA	-2.03	121.74	126.40
24	b	612	CLA	CGD-CBD-CAD	-2.03	104.15	110.73
33	l	101	LHG	C20-C19-C18	-2.03	104.11	114.42
24	c	509	CLA	C4D-C3D-CAD	-2.03	105.70	108.10
27	d	407	PL9	C12-C13-C14	-2.03	122.77	127.66
24	C	505	CLA	C6-C5-C3	2.03	118.78	113.45
32	b	621	LMG	C6-C5-C4	-2.03	108.25	113.00
24	b	613	CLA	O2D-CGD-O1D	-2.03	119.87	123.84
24	b	605	CLA	C16-C15-C13	-2.03	109.36	115.92
33	L	101	LHG	C27-C26-C25	-2.03	104.12	114.42
33	L	101	LHG	C20-C19-C18	-2.03	104.13	114.42
26	C	519	BCR	C27-C26-C25	2.03	125.68	122.73
24	D	404	CLA	C3D-C4D-ND	2.03	113.52	110.24
29	H	102	DGD	C7B-C6B-C5B	-2.03	104.14	114.42
24	c	502	CLA	C3A-C2A-C1A	2.03	104.37	101.34
24	C	503	CLA	C4D-C3D-CAD	-2.03	105.71	108.10
24	B	605	CLA	CHD-C4C-NC	2.03	127.39	124.20
24	B	607	CLA	CHB-C4A-NA	2.02	127.31	124.51
24	d	405	CLA	CHD-C4C-NC	2.02	127.39	124.20
24	b	617	CLA	C2C-C1C-NC	2.02	111.87	109.97
35	v	201	HEC	O1D-CGD-CBD	-2.02	116.58	123.08
24	D	404	CLA	C1D-ND-C4D	-2.02	104.90	106.33
24	B	609	CLA	CBC-CAC-C3C	-2.02	106.86	112.43
29	c	517	DGD	O6D-C1D-O3G	-2.02	105.19	109.97
29	c	516	DGD	C5B-C4B-C3B	-2.02	104.16	114.42
29	a	412	DGD	C1G-C2G-C3G	-2.02	107.07	111.80
33	D	411	LHG	O8-C6-C5	-2.02	102.55	108.43
32	b	623	LMG	C42-C41-C40	-2.02	104.17	114.42
26	b	602	BCR	C15-C16-C17	-2.02	119.34	123.47
24	b	612	CLA	CHA-C1A-NA	-2.02	121.77	126.40
27	A	410	PL9	C7-C3-C2	-2.02	120.64	123.30
32	c	522	LMG	O2-C2-C3	-2.02	105.68	110.35
26	b	618	BCR	C11-C10-C9	-2.02	124.43	127.31
28	f	101	SQD	O5-C1-O6	2.02	114.75	109.97
27	D	406	PL9	C8-C7-C3	2.02	117.68	111.98
29	C	517	DGD	O3G-C1D-C2D	-2.02	105.16	108.30
24	b	607	CLA	O1D-CGD-CBD	2.02	128.61	124.48
26	B	617	BCR	C37-C22-C21	-2.01	120.10	122.92
24	b	604	CLA	O1A-CGA-CBA	2.01	131.59	123.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	f	101	SQD	O8-S-O9	-2.01	106.36	111.27
24	c	503	CLA	C2C-C1C-NC	2.01	111.86	109.97
24	A	408	CLA	O1A-CGA-CBA	2.01	131.57	123.73
24	c	505	CLA	C1B-CHB-C4A	-2.01	126.14	130.12
26	C	515	BCR	C29-C30-C25	2.01	113.57	110.48
29	c	518	DGD	CDB-CCB-CBB	-2.01	104.23	114.42
26	B	619	BCR	C40-C30-C29	-2.01	100.87	108.91
24	b	607	CLA	CMD-C2D-C1D	2.01	128.25	124.71
28	a	410	SQD	C3-C4-C5	2.01	113.82	110.24
27	a	409	PL9	C35-C34-C36	2.01	118.65	115.27
24	h	101	CLA	CHD-C4C-NC	2.01	127.36	124.20
24	B	608	CLA	C6-C5-C3	-2.01	108.19	113.45
27	A	410	PL9	C12-C13-C14	-2.01	122.83	127.66
24	d	405	CLA	C3D-C4D-ND	2.01	113.48	110.24
24	b	613	CLA	C3D-C4D-ND	2.00	113.48	110.24
23	d	401	BCT	O3-C-O1	-2.00	114.35	119.55
24	b	611	CLA	C16-C17-C18	-2.00	106.54	115.98
24	c	504	CLA	CHD-C1D-ND	-2.00	122.61	124.45
24	C	506	CLA	C2D-C1D-ND	-2.00	108.63	110.10
24	B	610	CLA	O1A-CGA-CBA	2.00	131.54	123.73
29	c	518	DGD	CBB-CAB-C9B	-2.00	104.26	114.42
24	B	612	CLA	C1B-CHB-C4A	-2.00	126.15	130.12

All (61) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	A	405	CLA	ND
24	A	406	CLA	ND
24	A	408	CLA	ND
24	B	601	CLA	ND
24	B	602	CLA	ND
24	B	604	CLA	ND
24	B	605	CLA	ND
24	B	606	CLA	ND
24	B	607	CLA	ND
24	B	610	CLA	ND
24	B	612	CLA	ND
24	B	613	CLA	ND
24	B	614	CLA	ND
24	B	615	CLA	ND
24	B	616	CLA	ND
24	C	502	CLA	ND

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Mol	Chain	Res	Type	Atom
24	C	503	CLA	ND
24	C	504	CLA	ND
24	C	505	CLA	ND
24	C	506	CLA	ND
24	C	508	CLA	ND
24	C	510	CLA	ND
24	C	511	CLA	ND
24	C	512	CLA	ND
24	C	513	CLA	ND
24	C	514	CLA	ND
24	D	402	CLA	ND
24	D	403	CLA	ND
24	a	404	CLA	ND
24	a	407	CLA	ND
24	b	603	CLA	ND
24	b	604	CLA	ND
24	b	605	CLA	ND
24	b	606	CLA	ND
24	b	607	CLA	ND
24	b	608	CLA	ND
24	b	609	CLA	ND
24	b	610	CLA	ND
24	b	611	CLA	ND
24	b	612	CLA	ND
24	b	613	CLA	ND
24	b	614	CLA	ND
24	b	615	CLA	ND
24	b	616	CLA	ND
24	b	617	CLA	ND
24	c	501	CLA	ND
24	c	502	CLA	ND
24	c	503	CLA	ND
24	c	504	CLA	ND
24	c	505	CLA	ND
24	c	506	CLA	ND
24	c	507	CLA	ND
24	c	509	CLA	ND
24	c	510	CLA	ND
24	c	511	CLA	ND
24	c	512	CLA	ND
24	c	513	CLA	ND
24	d	403	CLA	ND

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Mol	Chain	Res	Type	Atom
24	d	404	CLA	ND
24	d	405	CLA	ND
24	h	101	CLA	ND

All (1710) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	408	CLA	C2-C3-C5-C6
24	A	408	CLA	C4-C3-C5-C6
24	B	605	CLA	C4-C3-C5-C6
24	B	606	CLA	CHA-CBD-CGD-O1D
24	B	616	CLA	CBD-CGD-O2D-CED
24	C	509	CLA	CHA-CBD-CGD-O1D
24	C	509	CLA	CHA-CBD-CGD-O2D
24	C	514	CLA	O2A-C1-C2-C3
24	D	402	CLA	CHA-CBD-CGD-O1D
24	D	402	CLA	CHA-CBD-CGD-O2D
24	b	606	CLA	C11-C10-C8-C9
24	b	607	CLA	CHA-CBD-CGD-O1D
24	b	615	CLA	CHA-CBD-CGD-O1D
24	b	615	CLA	CHA-CBD-CGD-O2D
24	b	615	CLA	CAD-CBD-CGD-O1D
24	b	615	CLA	CAD-CBD-CGD-O2D
24	b	617	CLA	CBD-CGD-O2D-CED
24	c	506	CLA	C4-C3-C5-C6
24	c	507	CLA	C4-C3-C5-C6
24	c	508	CLA	CHA-CBD-CGD-O1D
24	c	508	CLA	CHA-CBD-CGD-O2D
24	c	509	CLA	C11-C12-C13-C14
24	c	510	CLA	CBD-CGD-O2D-CED
26	A	409	BCR	C1-C6-C7-C8
26	A	409	BCR	C7-C8-C9-C10
26	A	409	BCR	C7-C8-C9-C34
26	A	409	BCR	C17-C18-C19-C20
26	B	617	BCR	C35-C13-C14-C15
26	B	619	BCR	C7-C8-C9-C34
26	B	619	BCR	C11-C12-C13-C35
26	C	515	BCR	C37-C22-C23-C24
26	C	519	BCR	C7-C8-C9-C10
26	C	519	BCR	C11-C12-C13-C35
26	C	519	BCR	C35-C13-C14-C15
26	C	519	BCR	C16-C17-C18-C36

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Mol	Chain	Res	Type	Atoms
26	D	405	BCR	C21-C22-C23-C24
26	D	405	BCR	C23-C24-C25-C26
26	D	405	BCR	C23-C24-C25-C30
26	K	101	BCR	C11-C10-C9-C8
26	K	101	BCR	C11-C12-C13-C14
26	K	101	BCR	C11-C12-C13-C35
26	K	101	BCR	C16-C17-C18-C19
26	K	101	BCR	C16-C17-C18-C36
26	K	101	BCR	C22-C23-C24-C25
26	Y	101	BCR	C5-C6-C7-C8
26	Y	101	BCR	C21-C22-C23-C24
26	Y	101	BCR	C37-C22-C23-C24
26	a	408	BCR	C20-C21-C22-C37
26	b	602	BCR	C1-C6-C7-C8
26	b	602	BCR	C5-C6-C7-C8
26	b	602	BCR	C7-C8-C9-C10
26	b	602	BCR	C7-C8-C9-C34
26	b	602	BCR	C11-C12-C13-C14
26	b	602	BCR	C37-C22-C23-C24
26	b	619	BCR	C37-C22-C23-C24
26	b	620	BCR	C11-C12-C13-C14
26	b	620	BCR	C11-C12-C13-C35
26	b	620	BCR	C37-C22-C23-C24
26	c	514	BCR	C11-C10-C9-C8
26	c	515	BCR	C7-C8-C9-C34
26	c	515	BCR	C16-C17-C18-C36
26	c	515	BCR	C18-C19-C20-C21
26	c	515	BCR	C20-C21-C22-C37
26	c	521	BCR	C6-C7-C8-C9
26	c	521	BCR	C35-C13-C14-C15
26	c	521	BCR	C36-C18-C19-C20
26	c	521	BCR	C18-C19-C20-C21
26	c	521	BCR	C20-C21-C22-C37
26	d	406	BCR	C18-C19-C20-C21
26	d	406	BCR	C21-C22-C23-C24
26	h	103	BCR	C11-C10-C9-C8
26	h	103	BCR	C16-C17-C18-C36
26	k	101	BCR	C7-C8-C9-C10
26	k	101	BCR	C7-C8-C9-C34
26	k	101	BCR	C17-C18-C19-C20
26	t	101	BCR	C7-C8-C9-C34
26	t	101	BCR	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
26	t	101	BCR	C12-C13-C14-C15
26	t	101	BCR	C16-C17-C18-C36
26	t	101	BCR	C20-C21-C22-C37
27	A	410	PL9	C9-C11-C12-C13
27	A	410	PL9	C12-C13-C14-C15
27	A	410	PL9	C12-C13-C14-C16
27	A	410	PL9	C19-C21-C22-C23
27	A	410	PL9	C22-C23-C24-C25
27	A	410	PL9	C22-C23-C24-C26
27	A	410	PL9	C37-C38-C39-C40
27	A	410	PL9	C37-C38-C39-C41
27	A	410	PL9	C43-C44-C46-C47
27	D	406	PL9	C32-C33-C34-C35
27	D	406	PL9	C32-C33-C34-C36
27	a	409	PL9	C22-C23-C24-C25
27	a	409	PL9	C22-C23-C24-C26
27	a	409	PL9	C30-C29-C31-C32
27	a	409	PL9	C32-C33-C34-C35
27	a	409	PL9	C33-C34-C36-C37
27	a	409	PL9	C37-C38-C39-C40
27	a	409	PL9	C42-C43-C44-C45
27	d	407	PL9	C32-C33-C34-C36
27	d	407	PL9	C37-C38-C39-C41
27	d	407	PL9	C42-C43-C44-C45
27	d	407	PL9	C42-C43-C44-C46
27	d	407	PL9	C47-C48-C49-C50
28	B	622	SQD	C2-C1-O6-C44
28	B	622	SQD	O5-C1-O6-C44
28	B	622	SQD	O49-C7-O47-C45
28	B	622	SQD	C8-C7-O47-C45
28	F	101	SQD	C45-C44-O6-C1
28	a	410	SQD	O47-C45-C46-O48
28	a	411	SQD	O6-C44-C45-O47
28	a	411	SQD	O49-C7-O47-C45
28	a	411	SQD	C8-C7-O47-C45
28	b	601	SQD	O10-C23-O48-C46
28	f	101	SQD	O5-C1-O6-C44
29	A	413	DGD	O1B-C1B-O2G-C2G
29	A	413	DGD	O2G-C2G-C3G-O3G
32	C	501	LMG	O9-C10-O7-C8
32	C	501	LMG	C11-C10-O7-C8
32	D	410	LMG	C11-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
32	K	102	LMG	C11-C10-O7-C8
32	b	623	LMG	C11-C10-O7-C8
32	c	522	LMG	O10-C28-O8-C9
32	c	524	LMG	O6-C1-O1-C7
32	c	524	LMG	O10-C28-O8-C9
33	D	408	LHG	O1-C1-C2-O2
33	D	408	LHG	C3-O3-P-O5
33	D	408	LHG	C4-O6-P-O4
33	E	101	LHG	O1-C1-C2-C3
33	E	101	LHG	C4-O6-P-O4
33	E	101	LHG	O10-C23-O8-C6
33	L	101	LHG	C3-O3-P-O4
33	L	101	LHG	C4-O6-P-O4
33	d	408	LHG	O1-C1-C2-C3
33	d	408	LHG	C3-O3-P-O5
33	d	409	LHG	O1-C1-C2-C3
33	d	409	LHG	C3-O3-P-O5
33	d	409	LHG	C4-O6-P-O4
33	d	410	LHG	O1-C1-C2-C3
33	e	101	LHG	C1-C2-C3-O3
33	e	101	LHG	C3-O3-P-O5
33	e	101	LHG	C4-O6-P-O5
33	e	101	LHG	O10-C23-O8-C6
24	h	101	CLA	O1D-CGD-O2D-CED
24	b	617	CLA	O1D-CGD-O2D-CED
24	c	510	CLA	O1D-CGD-O2D-CED
24	B	601	CLA	CBD-CGD-O2D-CED
24	C	502	CLA	CBD-CGD-O2D-CED
24	C	509	CLA	CBD-CGD-O2D-CED
24	C	510	CLA	CBD-CGD-O2D-CED
24	c	509	CLA	CBD-CGD-O2D-CED
24	c	513	CLA	CBD-CGD-O2D-CED
24	h	101	CLA	CBD-CGD-O2D-CED
24	B	601	CLA	O1D-CGD-O2D-CED
24	c	509	CLA	O1D-CGD-O2D-CED
24	B	616	CLA	O1D-CGD-O2D-CED
24	C	510	CLA	O1D-CGD-O2D-CED
28	a	411	SQD	C24-C23-O48-C46
28	b	601	SQD	C24-C23-O48-C46
32	c	524	LMG	C29-C28-O8-C9
33	E	101	LHG	C24-C23-O8-C6
33	e	101	LHG	C24-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
27	d	407	PL9	C47-C48-C49-C51
24	D	403	CLA	CBD-CGD-O2D-CED
24	a	405	CLA	CBD-CGD-O2D-CED
24	c	511	CLA	CBD-CGD-O2D-CED
25	d	402	PHO	CBD-CGD-O2D-CED
28	a	411	SQD	O10-C23-O48-C46
29	a	412	DGD	O1A-C1A-O1G-C1G
32	c	519	LMG	C11-C10-O7-C8
32	D	410	LMG	O9-C10-O7-C8
32	K	102	LMG	O9-C10-O7-C8
32	b	623	LMG	O9-C10-O7-C8
32	c	522	LMG	O9-C10-O7-C8
32	c	522	LMG	C4-C5-C6-O5
24	b	605	CLA	C3-C5-C6-C7
29	A	413	DGD	C2B-C1B-O2G-C2G
27	A	410	PL9	C40-C39-C41-C42
24	B	605	CLA	C2-C3-C5-C6
24	c	506	CLA	C2-C3-C5-C6
24	c	507	CLA	C2-C3-C5-C6
24	B	606	CLA	C2A-CAA-CBA-CGA
24	b	607	CLA	C2A-CAA-CBA-CGA
28	F	101	SQD	O10-C23-O48-C46
24	B	601	CLA	CBA-CGA-O2A-C1
28	f	101	SQD	C24-C23-O48-C46
29	a	412	DGD	C2A-C1A-O1G-C1G
32	c	522	LMG	C29-C28-O8-C9
27	A	410	PL9	C47-C48-C49-C50
24	c	501	CLA	CBD-CGD-O2D-CED
27	A	410	PL9	C32-C33-C34-C36
27	a	409	PL9	C32-C33-C34-C36
28	a	410	SQD	O10-C23-O48-C46
32	C	501	LMG	O10-C28-O8-C9
32	M	101	LMG	O10-C28-O8-C9
28	B	622	SQD	C45-C46-O48-C23
24	B	604	CLA	C13-C15-C16-C17
24	B	607	CLA	CBD-CGD-O2D-CED
24	B	614	CLA	CBD-CGD-O2D-CED
24	c	504	CLA	CBD-CGD-O2D-CED
24	c	512	CLA	CBD-CGD-O2D-CED
33	D	409	LHG	O2-C2-C3-O3
33	e	101	LHG	O2-C2-C3-O3
24	b	615	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
24	B	601	CLA	O1A-CGA-O2A-C1
24	D	403	CLA	O1D-CGD-O2D-CED
32	c	524	LMG	O6-C5-C6-O5
33	d	408	LHG	C28-C29-C30-C31
26	c	515	BCR	C14-C15-C16-C17
32	C	501	LMG	O6-C5-C6-O5
32	c	519	LMG	O6-C5-C6-O5
27	A	410	PL9	C47-C48-C49-C51
32	c	522	LMG	O6-C5-C6-O5
24	B	614	CLA	C4-C3-C5-C6
24	b	604	CLA	C4-C3-C5-C6
24	b	606	CLA	C4-C3-C5-C6
24	B	614	CLA	C2-C3-C5-C6
24	b	604	CLA	C2-C3-C5-C6
24	b	606	CLA	C2-C3-C5-C6
27	d	407	PL9	C38-C39-C41-C42
29	C	516	DGD	O6E-C5E-C6E-O5E
29	c	518	DGD	O1A-C1A-O1G-C1G
32	C	501	LMG	O6-C1-O1-C7
27	A	410	PL9	C29-C31-C32-C33
27	A	410	PL9	C44-C46-C47-C48
27	a	409	PL9	C24-C26-C27-C28
27	a	409	PL9	C44-C46-C47-C48
27	d	407	PL9	C44-C46-C47-C48
28	F	101	SQD	C24-C23-O48-C46
24	c	513	CLA	O1D-CGD-O2D-CED
27	D	406	PL9	C37-C38-C39-C40
24	C	502	CLA	O1D-CGD-O2D-CED
24	C	509	CLA	O1D-CGD-O2D-CED
29	a	412	DGD	O1B-C1B-O2G-C2G
25	d	402	PHO	O1D-CGD-O2D-CED
32	C	501	LMG	C29-C28-O8-C9
32	M	101	LMG	C29-C28-O8-C9
32	c	519	LMG	C29-C28-O8-C9
24	a	405	CLA	O1D-CGD-O2D-CED
32	c	524	LMG	C4-C5-C6-O5
24	B	611	CLA	C8-C10-C11-C12
24	B	612	CLA	C13-C15-C16-C17
33	D	408	LHG	O2-C2-C3-O3
28	f	101	SQD	C2-C1-O6-C44
32	c	524	LMG	C2-C1-O1-C7
28	B	622	SQD	O6-C44-C45-O47

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Mol	Chain	Res	Type	Atoms
28	a	410	SQD	O6-C44-C45-O47
27	A	410	PL9	C18-C19-C21-C22
24	B	605	CLA	C11-C10-C8-C9
24	B	607	CLA	C14-C13-C15-C16
24	C	503	CLA	C6-C7-C8-C9
24	C	508	CLA	C11-C10-C8-C9
24	C	509	CLA	C11-C12-C13-C14
24	C	513	CLA	C11-C10-C8-C9
24	b	611	CLA	C14-C13-C15-C16
24	b	615	CLA	C6-C7-C8-C9
24	b	617	CLA	C11-C10-C8-C9
24	c	509	CLA	C6-C7-C8-C9
24	c	510	CLA	C11-C10-C8-C9
24	c	511	CLA	C14-C13-C15-C16
24	h	101	CLA	C11-C10-C8-C9
25	A	407	PHO	C14-C13-C15-C16
24	c	511	CLA	O1D-CGD-O2D-CED
24	a	404	CLA	CBD-CGD-O2D-CED
26	C	519	BCR	C7-C8-C9-C34
26	K	101	BCR	C7-C8-C9-C34
26	b	602	BCR	C11-C12-C13-C35
26	d	406	BCR	C37-C22-C23-C24
26	t	101	BCR	C11-C12-C13-C35
29	c	517	DGD	C1B-C2B-C3B-C4B
33	e	101	LHG	C7-C8-C9-C10
29	C	518	DGD	O1A-C1A-O1G-C1G
24	B	608	CLA	C15-C16-C17-C18
24	B	612	CLA	C10-C11-C12-C13
24	b	612	CLA	C8-C10-C11-C12
24	c	503	CLA	C5-C6-C7-C8
24	h	101	CLA	C8-C10-C11-C12
29	H	102	DGD	O6E-C5E-C6E-O5E
28	F	101	SQD	C45-C46-O48-C23
32	K	102	LMG	C29-C28-O8-C9
24	D	404	CLA	C5-C6-C7-C8
24	c	506	CLA	C13-C15-C16-C17
24	c	511	CLA	C15-C16-C17-C18
29	C	517	DGD	C1B-C2B-C3B-C4B
32	D	410	LMG	C10-C11-C12-C13
24	A	405	CLA	C15-C16-C17-C18
24	B	614	CLA	C13-C15-C16-C17
24	C	506	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
24	C	510	CLA	C10-C11-C12-C13
24	b	614	CLA	C13-C15-C16-C17
24	c	512	CLA	C13-C15-C16-C17
29	H	102	DGD	C4E-C5E-C6E-O5E
27	a	409	PL9	C47-C48-C49-C50
33	E	101	LHG	O1-C1-C2-O2
28	A	411	SQD	C7-C8-C9-C10
28	A	411	SQD	C23-C24-C25-C26
28	B	622	SQD	C23-C24-C25-C26
29	H	102	DGD	C1A-C2A-C3A-C4A
32	c	524	LMG	C28-C29-C30-C31
32	d	411	LMG	C28-C29-C30-C31
33	L	101	LHG	C23-C24-C25-C26
33	d	408	LHG	C23-C24-C25-C26
33	e	101	LHG	C23-C24-C25-C26
24	B	602	CLA	C13-C15-C16-C17
24	C	506	CLA	C8-C10-C11-C12
24	b	608	CLA	C10-C11-C12-C13
24	b	610	CLA	C15-C16-C17-C18
24	b	607	CLA	C15-C16-C17-C18
24	c	509	CLA	C8-C10-C11-C12
24	b	615	CLA	C5-C6-C7-C8
24	h	101	CLA	C15-C16-C17-C18
24	c	504	CLA	O1D-CGD-O2D-CED
24	B	611	CLA	C12-C13-C15-C16
24	B	615	CLA	C11-C12-C13-C15
24	C	511	CLA	C6-C7-C8-C10
24	a	405	CLA	C6-C7-C8-C10
24	b	606	CLA	C11-C12-C13-C15
24	b	611	CLA	C12-C13-C15-C16
24	c	505	CLA	CBD-CGD-O2D-CED
24	C	513	CLA	C10-C11-C12-C13
24	a	407	CLA	C13-C15-C16-C17
24	b	612	CLA	C13-C15-C16-C17
28	F	101	SQD	O6-C44-C45-C46
26	b	620	BCR	C6-C7-C8-C9
29	c	517	DGD	O6E-C1E-O5D-C6D
27	a	409	PL9	C14-C16-C17-C18
27	a	409	PL9	C29-C31-C32-C33
27	a	409	PL9	C39-C41-C42-C43
32	b	621	LMG	C10-C11-C12-C13
26	c	514	BCR	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
26	c	521	BCR	C10-C11-C12-C13
26	d	406	BCR	C10-C11-C12-C13
26	h	103	BCR	C18-C19-C20-C21
24	B	605	CLA	C5-C6-C7-C8
24	B	609	CLA	C13-C15-C16-C17
24	c	509	CLA	C15-C16-C17-C18
28	a	410	SQD	C24-C23-O48-C46
33	l	101	LHG	C7-C8-C9-C10
24	C	508	CLA	C10-C11-C12-C13
24	b	616	CLA	C15-C16-C17-C18
33	E	101	LHG	C8-C7-O7-C5
29	C	518	DGD	C8A-C9A-CAA-CBA
24	B	611	CLA	C13-C15-C16-C17
24	C	507	CLA	C13-C15-C16-C17
24	a	407	CLA	C5-C6-C7-C8
24	c	503	CLA	C8-C10-C11-C12
24	c	505	CLA	C15-C16-C17-C18
24	c	506	CLA	C5-C6-C7-C8
33	D	408	LHG	C3-O3-P-O6
33	D	409	LHG	C3-O3-P-O6
33	d	409	LHG	C4-O6-P-O3
33	e	101	LHG	C4-O6-P-O3
33	l	101	LHG	C4-O6-P-O3
24	b	603	CLA	C3-C5-C6-C7
24	c	512	CLA	CBA-CGA-O2A-C1
24	b	610	CLA	CBD-CGD-O2D-CED
24	B	606	CLA	C15-C16-C17-C18
24	c	509	CLA	C10-C11-C12-C13
32	D	410	LMG	C28-C29-C30-C31
32	c	519	LMG	C28-C29-C30-C31
27	d	407	PL9	C40-C39-C41-C42
24	b	616	CLA	C16-C17-C18-C20
24	c	506	CLA	C16-C17-C18-C19
24	B	613	CLA	C5-C6-C7-C8
26	h	103	BCR	C14-C15-C16-C17
24	D	403	CLA	C2C-C3C-CAC-CBC
26	b	602	BCR	C9-C10-C11-C12
32	C	501	LMG	C4-C5-C6-O5
29	H	102	DGD	C4B-C5B-C6B-C7B
29	c	516	DGD	C4B-C5B-C6B-C7B
33	L	101	LHG	C27-C28-C29-C30
24	B	615	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
26	C	519	BCR	C11-C10-C9-C34
26	C	519	BCR	C20-C21-C22-C37
26	D	405	BCR	C20-C21-C22-C37
26	H	101	BCR	C16-C17-C18-C36
26	H	101	BCR	C20-C21-C22-C37
26	K	101	BCR	C20-C21-C22-C37
26	b	620	BCR	C20-C21-C22-C37
26	c	514	BCR	C11-C10-C9-C34
26	c	515	BCR	C35-C13-C14-C15
26	d	406	BCR	C16-C17-C18-C36
26	d	406	BCR	C20-C21-C22-C37
26	h	103	BCR	C11-C10-C9-C34
26	k	101	BCR	C16-C17-C18-C36
26	k	101	BCR	C20-C21-C22-C37
26	t	101	BCR	C11-C10-C9-C34
28	f	101	SQD	C32-C33-C34-C35
29	A	413	DGD	C4A-C5A-C6A-C7A
29	C	517	DGD	C6A-C7A-C8A-C9A
29	C	518	DGD	CCA-CDA-CEA-CFA
29	c	516	DGD	C5B-C6B-C7B-C8B
32	B	621	LMG	C14-C15-C16-C17
32	B	621	LMG	C29-C30-C31-C32
32	K	102	LMG	C32-C33-C34-C35
32	c	522	LMG	C32-C33-C34-C35
33	D	408	LHG	C12-C13-C14-C15
33	D	408	LHG	C15-C16-C17-C18
33	d	408	LHG	C16-C17-C18-C19
33	d	409	LHG	C26-C27-C28-C29
24	c	510	CLA	C16-C17-C18-C19
27	D	406	PL9	C47-C48-C49-C51
28	a	411	SQD	C12-C13-C14-C15
29	H	102	DGD	C3B-C4B-C5B-C6B
29	c	518	DGD	C8A-C9A-CAA-CBA
29	h	104	DGD	C2B-C3B-C4B-C5B
32	b	621	LMG	C31-C32-C33-C34
32	h	102	LMG	C11-C12-C13-C14
33	E	101	LHG	C9-C10-C11-C12
33	d	408	LHG	C32-C33-C34-C35
33	d	409	LHG	C29-C30-C31-C32
33	l	101	LHG	C9-C10-C11-C12
24	c	512	CLA	O1D-CGD-O2D-CED
24	B	607	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
32	b	621	LMG	C32-C33-C34-C35
33	D	411	LHG	C25-C26-C27-C28
33	e	101	LHG	C13-C14-C15-C16
32	D	407	LMG	C14-C15-C16-C17
32	c	524	LMG	C12-C13-C14-C15
33	D	408	LHG	C10-C11-C12-C13
33	D	411	LHG	C12-C13-C14-C15
33	E	101	LHG	C33-C34-C35-C36
29	A	413	DGD	O6D-C5D-C6D-O5D
28	A	412	SQD	C12-C13-C14-C15
28	a	410	SQD	C34-C35-C36-C37
29	c	518	DGD	CCB-CDB-CEB-CFB
32	h	102	LMG	C36-C37-C38-C39
24	d	404	CLA	C3-C5-C6-C7
28	A	412	SQD	C7-C8-C9-C10
26	B	617	BCR	C12-C13-C14-C15
26	B	619	BCR	C11-C10-C9-C8
26	B	619	BCR	C16-C17-C18-C19
26	K	101	BCR	C20-C21-C22-C23
26	a	408	BCR	C20-C21-C22-C23
26	b	620	BCR	C12-C13-C14-C15
26	c	514	BCR	C16-C17-C18-C19
26	c	515	BCR	C20-C21-C22-C23
26	d	406	BCR	C16-C17-C18-C19
26	h	103	BCR	C16-C17-C18-C19
26	t	101	BCR	C16-C17-C18-C19
29	C	517	DGD	C2E-C1E-O5D-C6D
29	c	517	DGD	C2E-C1E-O5D-C6D
29	C	516	DGD	CCB-CDB-CEB-CFB
29	a	412	DGD	C6A-C7A-C8A-C9A
29	c	518	DGD	CCA-CDA-CEA-CFA
32	c	522	LMG	C11-C12-C13-C14
32	d	411	LMG	C34-C35-C36-C37
33	d	410	LHG	C30-C31-C32-C33
33	e	101	LHG	C14-C15-C16-C17
24	c	512	CLA	O1A-CGA-O2A-C1
28	f	101	SQD	O10-C23-O48-C46
24	A	406	CLA	C16-C17-C18-C19
24	C	503	CLA	C16-C17-C18-C19
24	c	501	CLA	O1D-CGD-O2D-CED
24	b	610	CLA	C4-C3-C5-C6
29	A	413	DGD	C2B-C3B-C4B-C5B

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Mol	Chain	Res	Type	Atoms
29	c	518	DGD	C4B-C5B-C6B-C7B
32	D	407	LMG	C34-C35-C36-C37
32	M	101	LMG	C38-C39-C40-C41
33	d	408	LHG	C10-C11-C12-C13
33	e	101	LHG	C12-C13-C14-C15
24	B	604	CLA	C11-C12-C13-C14
24	c	509	CLA	C11-C10-C8-C9
24	c	512	CLA	C6-C7-C8-C9
24	c	512	CLA	C11-C12-C13-C14
29	h	104	DGD	C9A-CAA-CBA-CCA
32	b	623	LMG	C18-C19-C20-C21
32	d	411	LMG	C14-C15-C16-C17
24	c	513	CLA	C8-C10-C11-C12
29	h	104	DGD	O6E-C5E-C6E-O5E
26	h	103	BCR	C36-C18-C19-C20
29	C	518	DGD	C6B-C7B-C8B-C9B
32	D	407	LMG	C30-C31-C32-C33
33	L	101	LHG	C9-C10-C11-C12
33	L	101	LHG	C11-C12-C13-C14
33	D	408	LHG	O1-C1-C2-C3
33	D	411	LHG	O1-C1-C2-C3
24	C	503	CLA	C3-C5-C6-C7
24	b	607	CLA	C10-C11-C12-C13
28	b	601	SQD	C8-C7-O47-C45
32	D	407	LMG	C20-C21-C22-C23
32	D	410	LMG	C11-C12-C13-C14
33	D	409	LHG	C30-C31-C32-C33
32	M	101	LMG	C28-C29-C30-C31
32	b	623	LMG	C10-C11-C12-C13
33	D	411	LHG	C23-C24-C25-C26
28	A	411	SQD	C31-C32-C33-C34
28	A	412	SQD	C26-C27-C28-C29
28	B	622	SQD	C11-C12-C13-C14
28	B	622	SQD	C13-C14-C15-C16
28	b	601	SQD	C12-C13-C14-C15
29	C	518	DGD	C2A-C3A-C4A-C5A
29	a	412	DGD	C7B-C8B-C9B-CAB
29	c	516	DGD	C9A-CAA-CBA-CCA
29	h	104	DGD	C3A-C4A-C5A-C6A
32	C	501	LMG	C14-C15-C16-C17
32	C	501	LMG	C30-C31-C32-C33
32	D	407	LMG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
32	D	407	LMG	C35-C36-C37-C38
32	c	519	LMG	C39-C40-C41-C42
32	d	411	LMG	C39-C40-C41-C42
33	D	408	LHG	C34-C35-C36-C37
33	D	409	LHG	C11-C12-C13-C14
33	D	411	LHG	C11-C12-C13-C14
33	L	101	LHG	C30-C31-C32-C33
33	d	409	LHG	C34-C35-C36-C37
33	d	410	LHG	C27-C28-C29-C30
33	l	101	LHG	C27-C28-C29-C30
24	A	406	CLA	C16-C17-C18-C20
24	c	510	CLA	C16-C17-C18-C20
24	d	404	CLA	C16-C17-C18-C19
29	C	517	DGD	O6E-C1E-O5D-C6D
27	a	409	PL9	C19-C21-C22-C23
28	B	622	SQD	C17-C18-C19-C20
29	A	413	DGD	C5B-C6B-C7B-C8B
29	C	516	DGD	C2B-C3B-C4B-C5B
32	D	407	LMG	C18-C19-C20-C21
33	D	411	LHG	C14-C15-C16-C17
28	B	622	SQD	C26-C27-C28-C29
28	f	101	SQD	C28-C29-C30-C31
29	A	413	DGD	C4B-C5B-C6B-C7B
29	A	413	DGD	C8B-C9B-CAB-CBB
32	b	623	LMG	C11-C12-C13-C14
33	d	408	LHG	C29-C30-C31-C32
29	C	517	DGD	C8A-C9A-CAA-CBA
29	c	517	DGD	C7B-C8B-C9B-CAB
32	B	621	LMG	C16-C17-C18-C19
32	b	621	LMG	C17-C18-C19-C20
32	c	519	LMG	C36-C37-C38-C39
28	B	622	SQD	C33-C34-C35-C36
28	F	101	SQD	C25-C26-C27-C28
28	f	101	SQD	C24-C25-C26-C27
29	C	518	DGD	C5A-C6A-C7A-C8A
32	b	621	LMG	C29-C30-C31-C32
33	d	408	LHG	C31-C32-C33-C34
24	B	614	CLA	O1D-CGD-O2D-CED
24	c	512	CLA	C3A-C2A-CAA-CBA
24	h	101	CLA	C3A-C2A-CAA-CBA
24	a	404	CLA	C15-C16-C17-C18
24	b	609	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
27	a	409	PL9	C47-C48-C49-C51
28	F	101	SQD	C33-C34-C35-C36
29	a	412	DGD	C4A-C5A-C6A-C7A
29	c	518	DGD	C5B-C6B-C7B-C8B
32	c	519	LMG	C35-C36-C37-C38
32	c	522	LMG	C36-C37-C38-C39
32	h	102	LMG	C37-C38-C39-C40
33	D	409	LHG	C27-C28-C29-C30
33	d	409	LHG	C14-C15-C16-C17
33	e	101	LHG	C26-C27-C28-C29
24	C	503	CLA	C16-C17-C18-C20
24	b	608	CLA	C16-C17-C18-C20
24	b	610	CLA	C16-C17-C18-C19
24	b	616	CLA	C16-C17-C18-C19
24	c	507	CLA	C16-C17-C18-C20
28	A	411	SQD	C11-C12-C13-C14
29	A	413	DGD	CAA-CBA-CCA-CDA
29	A	413	DGD	CBB-CCB-CDB-CEB
32	b	623	LMG	C16-C17-C18-C19
28	f	101	SQD	C44-C45-C46-O48
32	c	522	LMG	O1-C7-C8-C9
32	C	501	LMG	C12-C13-C14-C15
24	B	604	CLA	O2A-C1-C2-C3
24	C	513	CLA	O2A-C1-C2-C3
24	h	101	CLA	O2A-C1-C2-C3
26	A	409	BCR	C14-C15-C16-C17
26	D	405	BCR	C14-C15-C16-C17
26	d	406	BCR	C14-C15-C16-C17
29	c	516	DGD	C1A-C2A-C3A-C4A
28	b	601	SQD	C13-C14-C15-C16
29	C	517	DGD	C6B-C7B-C8B-C9B
24	b	612	CLA	C4-C3-C5-C6
27	a	409	PL9	C15-C14-C16-C17
27	a	409	PL9	C40-C39-C41-C42
27	d	407	PL9	C15-C14-C16-C17
24	b	612	CLA	C2-C3-C5-C6
27	a	409	PL9	C13-C14-C16-C17
27	d	407	PL9	C28-C29-C31-C32
32	c	522	LMG	C11-C10-O7-C8
24	B	607	CLA	O1D-CGD-O2D-CED
28	a	410	SQD	C13-C14-C15-C16
29	h	104	DGD	C5B-C6B-C7B-C8B

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Mol	Chain	Res	Type	Atoms
33	d	408	LHG	C33-C34-C35-C36
32	c	519	LMG	C4-C5-C6-O5
33	d	409	LHG	O1-C1-C2-O2
24	B	615	CLA	C10-C11-C12-C13
29	c	518	DGD	C3A-C4A-C5A-C6A
32	M	101	LMG	C32-C33-C34-C35
32	M	101	LMG	C36-C37-C38-C39
32	b	623	LMG	C31-C32-C33-C34
24	D	404	CLA	C16-C17-C18-C19
29	C	517	DGD	C5A-C6A-C7A-C8A
24	b	617	CLA	C10-C11-C12-C13
28	A	412	SQD	C28-C29-C30-C31
29	C	516	DGD	C5B-C6B-C7B-C8B
32	c	524	LMG	C38-C39-C40-C41
24	C	513	CLA	C3-C5-C6-C7
32	B	621	LMG	C32-C33-C34-C35
32	B	621	LMG	C28-C29-C30-C31
32	c	522	LMG	C10-C11-C12-C13
33	E	101	LHG	C7-C8-C9-C10
24	c	508	CLA	C13-C15-C16-C17
28	A	411	SQD	C24-C25-C26-C27
29	a	412	DGD	C2A-C3A-C4A-C5A
32	b	623	LMG	C23-C24-C25-C26
32	c	524	LMG	C33-C34-C35-C36
32	h	102	LMG	C31-C32-C33-C34
33	l	101	LHG	C31-C32-C33-C34
33	E	101	LHG	O9-C7-O7-C5
24	B	612	CLA	C2-C1-O2A-CGA
24	c	506	CLA	C2-C1-O2A-CGA
28	A	411	SQD	C30-C31-C32-C33
28	A	412	SQD	C14-C15-C16-C17
29	c	516	DGD	C4A-C5A-C6A-C7A
24	B	613	CLA	C8-C10-C11-C12
24	C	514	CLA	C13-C15-C16-C17
24	b	605	CLA	C10-C11-C12-C13
32	c	519	LMG	O10-C28-O8-C9
28	A	411	SQD	C32-C33-C34-C35
28	F	101	SQD	C27-C28-C29-C30
29	h	104	DGD	C7B-C8B-C9B-CAB
29	h	104	DGD	CCB-CDB-CEB-CFB
32	C	501	LMG	C16-C17-C18-C19
26	A	409	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
26	H	101	BCR	C23-C24-C25-C26
26	H	101	BCR	C23-C24-C25-C30
26	Y	101	BCR	C1-C6-C7-C8
26	b	619	BCR	C23-C24-C25-C26
26	b	619	BCR	C23-C24-C25-C30
26	h	103	BCR	C23-C24-C25-C26
26	h	103	BCR	C23-C24-C25-C30
29	a	412	DGD	C5B-C6B-C7B-C8B
32	c	522	LMG	C34-C35-C36-C37
32	d	411	LMG	C13-C14-C15-C16
33	d	410	LHG	C29-C30-C31-C32
24	C	504	CLA	C5-C6-C7-C8
29	a	412	DGD	C2B-C1B-O2G-C2G
29	C	517	DGD	C9A-CAA-CBA-CCA
32	b	621	LMG	C28-C29-C30-C31
33	d	410	LHG	C23-C24-C25-C26
33	D	408	LHG	C11-C12-C13-C14
24	a	407	CLA	C10-C11-C12-C13
24	c	507	CLA	C8-C10-C11-C12
28	a	411	SQD	C10-C11-C12-C13
24	C	511	CLA	C4-C3-C5-C6
27	D	406	PL9	C30-C29-C31-C32
24	B	604	CLA	C11-C10-C8-C7
24	B	604	CLA	C11-C12-C13-C15
24	C	507	CLA	C2-C3-C5-C6
24	C	508	CLA	C11-C10-C8-C7
24	C	511	CLA	C2-C3-C5-C6
24	b	608	CLA	C6-C7-C8-C10
24	b	610	CLA	C2-C3-C5-C6
24	b	613	CLA	C12-C13-C15-C16
24	b	615	CLA	C6-C7-C8-C10
24	b	617	CLA	C11-C10-C8-C7
24	c	505	CLA	C11-C10-C8-C7
24	c	506	CLA	C11-C10-C8-C7
24	c	512	CLA	C11-C12-C13-C15
33	L	101	LHG	O10-C23-O8-C6
29	H	102	DGD	CCA-CDA-CEA-CFA
24	C	507	CLA	C15-C16-C17-C18
24	c	513	CLA	C16-C17-C18-C20
24	d	404	CLA	C16-C17-C18-C20
28	f	101	SQD	O49-C7-O47-C45
33	L	101	LHG	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
29	c	518	DGD	C2A-C1A-O1G-C1G
32	M	101	LMG	C12-C13-C14-C15
32	M	101	LMG	C13-C14-C15-C16
33	d	408	LHG	C17-C18-C19-C20
24	h	101	CLA	C2A-CAA-CBA-CGA
24	B	601	CLA	C10-C11-C12-C13
24	B	614	CLA	C8-C10-C11-C12
24	C	509	CLA	C13-C15-C16-C17
28	A	411	SQD	C28-C29-C30-C31
24	B	607	CLA	C15-C16-C17-C18
24	C	513	CLA	C15-C16-C17-C18
24	c	502	CLA	C15-C16-C17-C18
24	c	510	CLA	C10-C11-C12-C13
29	a	412	DGD	C8B-C9B-CAB-CBB
33	l	101	LHG	C13-C14-C15-C16
33	L	101	LHG	C18-C19-C20-C21
24	c	513	CLA	C5-C6-C7-C8
28	a	410	SQD	C26-C27-C28-C29
28	a	411	SQD	C18-C19-C20-C21
33	D	408	LHG	C25-C26-C27-C28
33	L	101	LHG	C31-C32-C33-C34
33	d	408	LHG	C7-C8-C9-C10
33	e	101	LHG	C8-C7-O7-C5
28	A	411	SQD	C26-C27-C28-C29
28	B	622	SQD	C31-C32-C33-C34
33	d	409	LHG	C28-C29-C30-C31
24	B	605	CLA	C15-C16-C17-C18
24	b	611	CLA	C15-C16-C17-C18
24	c	512	CLA	C5-C6-C7-C8
28	b	601	SQD	C10-C11-C12-C13
29	C	518	DGD	CBA-CCA-CDA-CEA
28	a	410	SQD	O49-C7-O47-C45
32	c	524	LMG	C30-C31-C32-C33
33	E	101	LHG	C15-C16-C17-C18
33	d	408	LHG	C15-C16-C17-C18
24	C	506	CLA	C10-C11-C12-C13
28	A	411	SQD	O6-C44-C45-O47
24	b	608	CLA	C16-C17-C18-C19
28	B	622	SQD	C34-C35-C36-C37
32	b	623	LMG	O6-C5-C6-O5
27	D	406	PL9	C38-C39-C41-C42
27	d	407	PL9	C33-C34-C36-C37

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Mol	Chain	Res	Type	Atoms
27	d	407	PL9	C4-C3-C7-C8
29	c	516	DGD	C2A-C3A-C4A-C5A
32	D	407	LMG	C19-C20-C21-C22
33	E	101	LHG	C11-C10-C9-C8
24	B	604	CLA	C11-C10-C8-C9
24	B	605	CLA	C11-C12-C13-C14
24	B	615	CLA	C11-C12-C13-C14
24	C	509	CLA	C11-C10-C8-C9
24	C	511	CLA	C6-C7-C8-C9
24	C	511	CLA	C11-C10-C8-C9
24	a	405	CLA	C6-C7-C8-C9
24	b	605	CLA	C11-C10-C8-C9
24	b	606	CLA	C11-C12-C13-C14
24	b	608	CLA	C6-C7-C8-C9
24	b	613	CLA	C14-C13-C15-C16
24	c	505	CLA	C11-C10-C8-C9
24	c	506	CLA	C11-C10-C8-C9
24	c	508	CLA	C14-C13-C15-C16
24	b	615	CLA	CBD-CGD-O2D-CED
28	F	101	SQD	C26-C27-C28-C29
24	C	507	CLA	C3-C5-C6-C7
24	c	506	CLA	C3-C5-C6-C7
29	C	517	DGD	C3B-C4B-C5B-C6B
32	C	501	LMG	C39-C40-C41-C42
32	c	522	LMG	C40-C41-C42-C43
24	C	509	CLA	C1A-C2A-CAA-CBA
24	C	512	CLA	C1A-C2A-CAA-CBA
24	a	407	CLA	C1A-C2A-CAA-CBA
24	h	101	CLA	C1A-C2A-CAA-CBA
24	B	609	CLA	C16-C17-C18-C20
24	c	506	CLA	C16-C17-C18-C20
29	A	413	DGD	CDB-CEB-CFB-CGB
29	C	518	DGD	CAA-CBA-CCA-CDA
32	c	522	LMG	C38-C39-C40-C41
33	d	410	LHG	C32-C33-C34-C35
33	l	101	LHG	C16-C17-C18-C19
24	C	511	CLA	C10-C11-C12-C13
24	b	616	CLA	C8-C10-C11-C12
33	e	101	LHG	C3-O3-P-O6
32	D	407	LMG	C13-C14-C15-C16
24	b	616	CLA	C5-C6-C7-C8
33	E	101	LHG	O6-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
33	l	101	LHG	O6-C4-C5-C6
24	C	505	CLA	C11-C12-C13-C14
28	a	411	SQD	C11-C12-C13-C14
29	A	413	DGD	C8A-C9A-CAA-CBA
32	b	621	LMG	C37-C38-C39-C40
32	h	102	LMG	C32-C33-C34-C35
33	d	409	LHG	C11-C12-C13-C14
29	H	102	DGD	C9B-CAB-CBB-CCB
33	D	411	LHG	C10-C11-C12-C13
32	D	407	LMG	O6-C5-C6-O5
24	B	602	CLA	C8-C10-C11-C12
24	b	610	CLA	C16-C17-C18-C20
29	h	104	DGD	C7A-C8A-C9A-CAA
32	M	101	LMG	C14-C15-C16-C17
28	B	622	SQD	C9-C10-C11-C12
24	B	616	CLA	C5-C6-C7-C8
24	b	604	CLA	C8-C10-C11-C12
24	c	510	CLA	C15-C16-C17-C18
28	b	601	SQD	O49-C7-O47-C45
24	C	507	CLA	C4-C3-C5-C6
27	A	410	PL9	C30-C29-C31-C32
32	h	102	LMG	C33-C34-C35-C36
24	a	405	CLA	C8-C10-C11-C12
24	b	617	CLA	C5-C6-C7-C8
33	D	411	LHG	C27-C28-C29-C30
32	c	519	LMG	C31-C32-C33-C34
24	B	609	CLA	C16-C17-C18-C19
28	A	411	SQD	O6-C44-C45-C46
28	B	622	SQD	O6-C44-C45-C46
28	a	410	SQD	C12-C13-C14-C15
28	a	411	SQD	C44-C45-C46-O48
28	b	601	SQD	C44-C45-C46-O48
29	A	413	DGD	C1G-C2G-C3G-O3G
29	C	516	DGD	O1G-C1G-C2G-C3G
32	c	522	LMG	C7-C8-C9-O8
24	c	504	CLA	C5-C6-C7-C8
24	c	510	CLA	C8-C10-C11-C12
24	A	408	CLA	C6-C7-C8-C9
28	a	411	SQD	C15-C16-C17-C18
29	a	412	DGD	C3B-C4B-C5B-C6B
33	E	101	LHG	C27-C28-C29-C30
28	B	622	SQD	C45-C44-O6-C1

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Mol	Chain	Res	Type	Atoms
29	C	517	DGD	C2G-C3G-O3G-C1D
29	C	517	DGD	C5D-C6D-O5D-C1E
29	c	517	DGD	C2G-C3G-O3G-C1D
29	c	517	DGD	C5D-C6D-O5D-C1E
29	A	413	DGD	CEA-CFA-CGA-CHA
32	d	411	LMG	C15-C16-C17-C18
32	h	102	LMG	C29-C30-C31-C32
33	e	101	LHG	C17-C18-C19-C20
33	l	101	LHG	C29-C30-C31-C32
24	B	603	CLA	C10-C11-C12-C13
24	B	606	CLA	C8-C10-C11-C12
29	A	413	DGD	C4D-C5D-C6D-O5D
28	A	411	SQD	C15-C16-C17-C18
24	B	601	CLA	C3-C5-C6-C7
24	B	608	CLA	C5-C6-C7-C8
27	d	407	PL9	C34-C36-C37-C38
33	D	409	LHG	C17-C18-C19-C20
33	d	408	LHG	O1-C1-C2-O2
33	E	101	LHG	C24-C25-C26-C27
33	E	101	LHG	C35-C36-C37-C38
29	H	102	DGD	CBA-CCA-CDA-CEA
29	c	516	DGD	C8B-C9B-CAB-CBB
32	h	102	LMG	C28-C29-C30-C31
32	h	102	LMG	C39-C40-C41-C42
26	Y	101	BCR	C11-C10-C9-C34
29	C	517	DGD	O6E-C5E-C6E-O5E
29	c	516	DGD	O6E-C5E-C6E-O5E
32	d	411	LMG	O6-C5-C6-O5
24	B	615	CLA	C4-C3-C5-C6
29	A	413	DGD	CFA-CGA-CHA-CIA
24	B	601	CLA	C16-C17-C18-C20
24	c	512	CLA	C16-C17-C18-C19
24	C	512	CLA	CBA-CGA-O2A-C1
28	a	411	SQD	C19-C20-C21-C22
29	h	104	DGD	CAB-CBB-CCB-CDB
33	L	101	LHG	C32-C33-C34-C35
33	e	101	LHG	C28-C29-C30-C31
28	b	601	SQD	C46-C45-O47-C7
32	D	410	LMG	C9-C8-O7-C10
24	c	512	CLA	C2A-CAA-CBA-CGA
24	B	601	CLA	C2-C1-O2A-CGA
29	c	517	DGD	C6A-C7A-C8A-C9A

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Mol	Chain	Res	Type	Atoms
29	h	104	DGD	CDA-CEA-CFA-CGA
32	d	411	LMG	C30-C31-C32-C33
33	d	410	LHG	C25-C26-C27-C28
24	c	508	CLA	C15-C16-C17-C18
29	a	412	DGD	CFA-CGA-CHA-CIA
32	D	407	LMG	C33-C34-C35-C36
33	D	409	LHG	C9-C10-C11-C12
33	d	409	LHG	C33-C34-C35-C36
24	B	611	CLA	CBA-CGA-O2A-C1
29	A	413	DGD	C1A-C2A-C3A-C4A
28	A	412	SQD	C30-C31-C32-C33
29	A	413	DGD	CDA-CEA-CFA-CGA
32	K	102	LMG	C30-C31-C32-C33
33	D	411	LHG	C18-C19-C20-C21
33	l	101	LHG	C24-C25-C26-C27
28	b	601	SQD	C19-C20-C21-C22
32	b	621	LMG	C19-C20-C21-C22
24	b	606	CLA	C15-C16-C17-C18
24	b	615	CLA	C15-C16-C17-C18
24	a	404	CLA	O1D-CGD-O2D-CED
26	C	519	BCR	C12-C13-C14-C15
26	d	406	BCR	C11-C10-C9-C8
28	b	601	SQD	O6-C44-C45-O47
32	c	522	LMG	O1-C7-C8-O7
28	a	411	SQD	C31-C32-C33-C34
29	a	412	DGD	C8A-C9A-CAA-CBA
29	c	517	DGD	CDA-CEA-CFA-CGA
33	d	408	LHG	C19-C20-C21-C22
24	h	101	CLA	C10-C11-C12-C13
33	E	101	LHG	C19-C20-C21-C22
24	B	605	CLA	C11-C12-C13-C15
24	B	606	CLA	C6-C7-C8-C10
24	B	615	CLA	C6-C7-C8-C10
24	C	507	CLA	C12-C13-C15-C16
24	C	509	CLA	C11-C10-C8-C7
24	C	511	CLA	C11-C10-C8-C7
24	a	405	CLA	C11-C10-C8-C7
24	a	405	CLA	C12-C13-C15-C16
24	a	407	CLA	C11-C10-C8-C7
24	b	605	CLA	C11-C10-C8-C7
24	b	607	CLA	C11-C10-C8-C7
24	b	608	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
24	b	609	CLA	C11-C10-C8-C7
24	b	615	CLA	C11-C12-C13-C15
24	b	616	CLA	C12-C13-C15-C16
24	c	508	CLA	C12-C13-C15-C16
24	c	510	CLA	C11-C10-C8-C7
25	A	407	PHO	C12-C13-C15-C16
27	D	406	PL9	C28-C29-C31-C32
24	B	611	CLA	O1A-CGA-O2A-C1
28	A	412	SQD	C34-C35-C36-C37
24	B	611	CLA	C11-C12-C13-C14
24	B	611	CLA	C14-C13-C15-C16
24	B	614	CLA	C14-C13-C15-C16
24	C	507	CLA	C14-C13-C15-C16
24	C	508	CLA	C14-C13-C15-C16
24	a	405	CLA	C11-C10-C8-C9
24	a	405	CLA	C14-C13-C15-C16
24	a	407	CLA	C11-C10-C8-C9
24	b	603	CLA	C6-C7-C8-C9
24	b	607	CLA	C11-C10-C8-C9
24	b	610	CLA	C14-C13-C15-C16
24	b	616	CLA	C11-C10-C8-C9
24	b	616	CLA	C14-C13-C15-C16
24	d	404	CLA	C6-C7-C8-C9
28	f	101	SQD	C31-C32-C33-C34
32	d	411	LMG	C35-C36-C37-C38
29	C	517	DGD	CDA-CEA-CFA-CGA
29	h	104	DGD	C3B-C4B-C5B-C6B
32	b	621	LMG	C13-C14-C15-C16
26	c	515	BCR	C21-C22-C23-C24
28	A	412	SQD	C10-C11-C12-C13
29	C	518	DGD	C3A-C4A-C5A-C6A
33	L	101	LHG	C26-C27-C28-C29
24	B	605	CLA	C10-C11-C12-C13
32	D	410	LMG	C37-C38-C39-C40
32	c	519	LMG	C38-C39-C40-C41
28	B	622	SQD	C24-C23-O48-C46
33	D	408	LHG	C33-C34-C35-C36
28	F	101	SQD	C23-C24-C25-C26
33	D	409	LHG	C23-C24-C25-C26
24	b	608	CLA	C8-C10-C11-C12
24	c	511	CLA	C13-C15-C16-C17
24	B	613	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
32	D	407	LMG	C40-C41-C42-C43
33	E	101	LHG	C16-C17-C18-C19
26	B	617	BCR	C6-C7-C8-C9
24	B	613	CLA	CBD-CGD-O2D-CED
24	b	610	CLA	O1D-CGD-O2D-CED
29	H	102	DGD	C7A-C8A-C9A-CAA
32	c	524	LMG	C32-C33-C34-C35
32	c	524	LMG	C16-C17-C18-C19
24	B	604	CLA	C10-C11-C12-C13
24	D	402	CLA	C15-C16-C17-C18
24	b	611	CLA	C8-C10-C11-C12
24	d	405	CLA	C8-C10-C11-C12
29	c	518	DGD	C7A-C8A-C9A-CAA
32	c	524	LMG	C39-C40-C41-C42
24	C	505	CLA	C4-C3-C5-C6
24	B	615	CLA	C2-C3-C5-C6
27	a	409	PL9	C38-C39-C41-C42
32	M	101	LMG	O9-C10-O7-C8
32	M	101	LMG	C15-C16-C17-C18
33	L	101	LHG	C19-C20-C21-C22
24	C	510	CLA	C16-C17-C18-C19
24	C	510	CLA	C16-C17-C18-C20
24	a	404	CLA	C16-C17-C18-C20
26	c	514	BCR	C13-C14-C15-C16
33	E	101	LHG	C30-C31-C32-C33
29	A	413	DGD	CEB-CFB-CGB-CHB
29	c	516	DGD	CAB-CBB-CCB-CDB
32	D	410	LMG	C33-C34-C35-C36
24	B	610	CLA	C16-C17-C18-C19
29	C	518	DGD	C2A-C1A-O1G-C1G
24	c	508	CLA	C16-C17-C18-C19
28	A	412	SQD	C44-C45-C46-O48
28	a	410	SQD	O6-C44-C45-C46
28	a	410	SQD	C44-C45-C46-O48
32	D	410	LMG	C7-C8-C9-O8
28	f	101	SQD	C25-C26-C27-C28
29	c	516	DGD	C3A-C4A-C5A-C6A
29	c	517	DGD	CAB-CBB-CCB-CDB
33	E	101	LHG	C23-C24-C25-C26
24	C	512	CLA	O1A-CGA-O2A-C1
33	d	410	LHG	C26-C27-C28-C29
29	C	516	DGD	O6D-C5D-C6D-O5D

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Mol	Chain	Res	Type	Atoms
32	c	524	LMG	C14-C15-C16-C17
33	D	409	LHG	C25-C26-C27-C28
28	A	411	SQD	C13-C14-C15-C16
29	C	516	DGD	CDA-CEA-CFA-CGA
29	C	517	DGD	C7A-C8A-C9A-CAA
32	C	501	LMG	C32-C33-C34-C35
24	b	603	CLA	C16-C17-C18-C20
24	h	101	CLA	C16-C17-C18-C20
28	A	411	SQD	C11-C10-C9-C8
28	B	622	SQD	C25-C26-C27-C28
28	a	410	SQD	C10-C11-C12-C13
32	B	621	LMG	C35-C36-C37-C38
32	D	410	LMG	C12-C13-C14-C15
32	D	410	LMG	C14-C15-C16-C17
32	b	621	LMG	C4-C5-C6-O5
33	D	408	LHG	C4-O6-P-O3
33	E	101	LHG	C4-O6-P-O3
33	d	408	LHG	C3-O3-P-O6
32	C	501	LMG	C10-C11-C12-C13
32	K	102	LMG	O10-C28-O8-C9
32	c	519	LMG	O9-C10-O7-C8
28	A	411	SQD	C14-C15-C16-C17
32	b	623	LMG	C19-C20-C21-C22
33	e	101	LHG	C27-C28-C29-C30
33	e	101	LHG	O6-C4-C5-O7
29	c	516	DGD	O1B-C1B-O2G-C2G
24	c	506	CLA	CBA-CGA-O2A-C1
24	c	513	CLA	C16-C17-C18-C19
33	D	408	LHG	C29-C30-C31-C32
28	F	101	SQD	O48-C23-C24-C25
28	f	101	SQD	C33-C34-C35-C36
29	C	517	DGD	C3A-C4A-C5A-C6A
24	b	606	CLA	C10-C11-C12-C13
28	A	412	SQD	O47-C45-C46-O48
32	M	101	LMG	C40-C41-C42-C43
32	c	522	LMG	C12-C13-C14-C15
28	a	411	SQD	O47-C45-C46-O48
32	M	101	LMG	O7-C8-C9-O8
32	c	522	LMG	O7-C8-C9-O8
33	D	409	LHG	C24-C25-C26-C27
24	B	610	CLA	C16-C17-C18-C20
24	B	612	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
24	B	615	CLA	C16-C17-C18-C19
24	B	616	CLA	C11-C12-C13-C14
28	a	411	SQD	O6-C44-C45-C46
33	D	408	LHG	C1-C2-C3-O3
33	D	409	LHG	C1-C2-C3-O3
24	C	507	CLA	C2-C1-O2A-CGA
24	c	510	CLA	C2-C1-O2A-CGA
29	c	516	DGD	CCB-CDB-CEB-CFB
32	D	410	LMG	C34-C35-C36-C37
24	B	615	CLA	C6-C7-C8-C9
24	C	506	CLA	C11-C12-C13-C14
24	C	507	CLA	C6-C7-C8-C9
24	C	514	CLA	C11-C10-C8-C9
24	b	609	CLA	C11-C12-C13-C14
24	b	614	CLA	C6-C7-C8-C9
24	b	614	CLA	C11-C12-C13-C14
24	b	615	CLA	C11-C12-C13-C14
24	c	506	CLA	C6-C7-C8-C9
24	d	405	CLA	C11-C12-C13-C14
28	a	411	SQD	C13-C14-C15-C16
32	d	411	LMG	C38-C39-C40-C41
33	D	411	LHG	C11-C10-C9-C8
24	B	601	CLA	C16-C17-C18-C19
24	a	404	CLA	C16-C17-C18-C19
24	c	512	CLA	C16-C17-C18-C20
26	B	619	BCR	C5-C6-C7-C8
26	C	519	BCR	C23-C24-C25-C26
26	C	519	BCR	C23-C24-C25-C30
26	Y	101	BCR	C23-C24-C25-C30
26	b	618	BCR	C5-C6-C7-C8
26	c	521	BCR	C1-C6-C7-C8
26	c	521	BCR	C5-C6-C7-C8
26	c	521	BCR	C23-C24-C25-C26
26	k	101	BCR	C1-C6-C7-C8
29	H	102	DGD	O2G-C1B-C2B-C3B
26	a	408	BCR	C21-C22-C23-C24
26	b	619	BCR	C21-C22-C23-C24
26	h	103	BCR	C17-C18-C19-C20
24	B	610	CLA	C8-C10-C11-C12
24	c	507	CLA	C5-C6-C7-C8
32	c	522	LMG	C31-C32-C33-C34
27	D	406	PL9	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
28	b	601	SQD	C16-C17-C18-C19
24	D	404	CLA	C16-C17-C18-C20
24	b	603	CLA	C16-C17-C18-C19
24	c	507	CLA	C16-C17-C18-C19
32	c	524	LMG	C35-C36-C37-C38
29	c	516	DGD	O6D-C5D-C6D-O5D
24	c	510	CLA	C4-C3-C5-C6
33	D	409	LHG	C31-C32-C33-C34
33	D	409	LHG	C35-C36-C37-C38
24	B	603	CLA	C6-C7-C8-C10
24	B	605	CLA	C11-C10-C8-C7
24	B	616	CLA	C6-C7-C8-C10
24	C	505	CLA	C11-C10-C8-C7
24	C	506	CLA	C11-C12-C13-C15
24	C	513	CLA	C12-C13-C15-C16
24	C	514	CLA	C11-C10-C8-C7
24	C	514	CLA	C12-C13-C15-C16
24	D	404	CLA	C11-C10-C8-C7
24	D	404	CLA	C12-C13-C15-C16
24	b	603	CLA	C6-C7-C8-C10
24	b	609	CLA	C11-C12-C13-C15
24	b	610	CLA	C12-C13-C15-C16
24	b	616	CLA	C11-C10-C8-C7
24	c	501	CLA	C11-C12-C13-C15
24	c	509	CLA	C11-C12-C13-C15
24	d	404	CLA	C6-C7-C8-C10
24	h	101	CLA	C11-C12-C13-C15
32	b	623	LMG	C15-C16-C17-C18
24	b	608	CLA	C5-C6-C7-C8
26	K	101	BCR	C9-C10-C11-C12
26	c	514	BCR	C15-C16-C17-C18
26	k	101	BCR	C19-C20-C21-C22
29	C	518	DGD	C4B-C5B-C6B-C7B
24	b	615	CLA	C8-C10-C11-C12
26	B	617	BCR	C16-C17-C18-C36
26	K	101	BCR	C11-C10-C9-C34
26	b	618	BCR	C35-C13-C14-C15
26	b	620	BCR	C35-C13-C14-C15
26	c	514	BCR	C16-C17-C18-C36
32	M	101	LMG	O6-C5-C6-O5
32	K	102	LMG	C28-C29-C30-C31
24	B	616	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
24	C	503	CLA	CBA-CGA-O2A-C1
28	a	410	SQD	C9-C10-C11-C12
28	B	622	SQD	C24-C25-C26-C27
32	C	501	LMG	C38-C39-C40-C41
24	A	405	CLA	CAD-CBD-CGD-O2D
24	B	604	CLA	CAD-CBD-CGD-O2D
24	B	616	CLA	CAD-CBD-CGD-O2D
24	C	506	CLA	CAD-CBD-CGD-O2D
24	C	511	CLA	CAD-CBD-CGD-O2D
24	D	404	CLA	CAD-CBD-CGD-O2D
24	a	404	CLA	CAD-CBD-CGD-O2D
24	b	617	CLA	CAD-CBD-CGD-O2D
24	c	501	CLA	CAD-CBD-CGD-O2D
24	c	503	CLA	CAD-CBD-CGD-O2D
25	A	407	PHO	CAD-CBD-CGD-O2D
25	a	406	PHO	CAD-CBD-CGD-O2D
32	b	621	LMG	C11-C12-C13-C14
24	B	608	CLA	C13-C15-C16-C17
24	b	612	CLA	C10-C11-C12-C13
24	c	506	CLA	C15-C16-C17-C18
29	C	516	DGD	O1G-C1A-C2A-C3A
26	C	519	BCR	C6-C7-C8-C9
26	c	514	BCR	C22-C23-C24-C25
32	C	501	LMG	C35-C36-C37-C38
32	c	524	LMG	C11-C12-C13-C14
28	F	101	SQD	O5-C1-O6-C44
29	a	412	DGD	O1G-C1G-C2G-C3G
32	M	101	LMG	C7-C8-C9-O8
33	d	410	LHG	C2-C3-O3-P
33	D	409	LHG	O6-C4-C5-O7
33	E	101	LHG	O6-C4-C5-O7
24	B	607	CLA	C10-C11-C12-C13
24	C	513	CLA	C8-C10-C11-C12
34	e	102	HEM	C4B-C3B-CAB-CBB
33	e	101	LHG	C16-C17-C18-C19
24	B	614	CLA	CHA-CBD-CGD-O1D
24	B	614	CLA	CHA-CBD-CGD-O2D
24	C	503	CLA	CHA-CBD-CGD-O1D
24	C	503	CLA	CHA-CBD-CGD-O2D
24	C	505	CLA	CHA-CBD-CGD-O1D
24	C	505	CLA	CHA-CBD-CGD-O2D
24	C	513	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
24	c	502	CLA	CHA-CBD-CGD-O1D
24	c	502	CLA	CHA-CBD-CGD-O2D
24	c	504	CLA	CHA-CBD-CGD-O1D
24	c	504	CLA	CHA-CBD-CGD-O2D
24	c	507	CLA	CHA-CBD-CGD-O1D
24	c	507	CLA	CHA-CBD-CGD-O2D
24	c	509	CLA	CHA-CBD-CGD-O1D
24	c	509	CLA	CHA-CBD-CGD-O2D
24	c	510	CLA	CHA-CBD-CGD-O1D
24	h	101	CLA	CHA-CBD-CGD-O1D
24	h	101	CLA	CHA-CBD-CGD-O2D
32	b	621	LMG	O10-C28-O8-C9
29	h	104	DGD	C8B-C9B-CAB-CBB
26	H	101	BCR	C11-C10-C9-C8
26	b	602	BCR	C20-C21-C22-C23
29	h	104	DGD	C6A-C7A-C8A-C9A
32	D	410	LMG	C36-C37-C38-C39
29	a	412	DGD	O1G-C1G-C2G-O2G
32	D	410	LMG	O7-C8-C9-O8
29	h	104	DGD	CCA-CDA-CEA-CFA
24	b	608	CLA	CBD-CGD-O2D-CED
24	c	506	CLA	O1A-CGA-O2A-C1
29	C	516	DGD	C2A-C3A-C4A-C5A
33	d	410	LHG	O1-C1-C2-O2
28	A	412	SQD	C11-C12-C13-C14
29	c	518	DGD	C1A-C2A-C3A-C4A
24	c	510	CLA	C2-C3-C5-C6
27	D	406	PL9	C4-C3-C7-C8
27	a	409	PL9	C4-C3-C7-C8
24	C	511	CLA	C15-C16-C17-C18
24	C	513	CLA	C14-C13-C15-C16
24	C	514	CLA	C14-C13-C15-C16
24	D	404	CLA	C11-C10-C8-C9
24	b	604	CLA	C11-C12-C13-C14
24	b	607	CLA	C14-C13-C15-C16
28	A	412	SQD	C46-C45-O47-C7
33	D	409	LHG	C29-C30-C31-C32
28	b	601	SQD	C24-C25-C26-C27
29	A	413	DGD	CBA-CCA-CDA-CEA
26	b	618	BCR	C11-C12-C13-C35
26	b	619	BCR	C7-C8-C9-C34
32	D	410	LMG	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
32	c	524	LMG	C40-C41-C42-C43
28	a	410	SQD	C30-C31-C32-C33
24	c	512	CLA	C1A-C2A-CAA-CBA
29	c	517	DGD	C1A-C2A-C3A-C4A
24	C	511	CLA	C16-C17-C18-C20
24	h	101	CLA	C16-C17-C18-C19
29	C	517	DGD	C5B-C6B-C7B-C8B
33	l	101	LHG	C34-C35-C36-C37
24	B	603	CLA	C13-C15-C16-C17
33	d	409	LHG	C3-O3-P-O6
29	a	412	DGD	C5A-C6A-C7A-C8A
32	h	102	LMG	C35-C36-C37-C38
29	C	516	DGD	C4D-C5D-C6D-O5D
29	c	516	DGD	C4D-C5D-C6D-O5D
33	E	101	LHG	C2-C3-O3-P
24	b	608	CLA	O1A-CGA-O2A-C1
33	D	408	LHG	C3-O3-P-O4
33	D	409	LHG	C3-O3-P-O5
33	e	101	LHG	C4-O6-P-O4
33	l	101	LHG	C4-O6-P-O5
24	B	615	CLA	C16-C17-C18-C20
24	a	405	CLA	C16-C17-C18-C20
28	A	412	SQD	C24-C23-O48-C46
29	H	102	DGD	C3A-C4A-C5A-C6A
32	M	101	LMG	C19-C20-C21-C22
29	C	516	DGD	C4E-C5E-C6E-O5E
24	B	616	CLA	C3-C5-C6-C7
33	E	101	LHG	C28-C29-C30-C31
28	A	411	SQD	C25-C26-C27-C28
32	b	623	LMG	C35-C36-C37-C38
24	B	601	CLA	CAD-CBD-CGD-O1D
24	B	614	CLA	CAD-CBD-CGD-O1D
24	C	503	CLA	CAD-CBD-CGD-O1D
24	C	505	CLA	CAD-CBD-CGD-O1D
24	C	514	CLA	CAD-CBD-CGD-O1D
24	c	502	CLA	CAD-CBD-CGD-O1D
24	c	504	CLA	CAD-CBD-CGD-O1D
24	h	101	CLA	CAD-CBD-CGD-O1D
32	D	407	LMG	C28-C29-C30-C31
24	C	512	CLA	C8-C10-C11-C12
24	C	509	CLA	C2C-C3C-CAC-CBC
33	D	409	LHG	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
32	C	501	LMG	C19-C20-C21-C22
24	b	614	CLA	C8-C10-C11-C12
32	d	411	LMG	C33-C34-C35-C36
32	h	102	LMG	C38-C39-C40-C41
24	B	602	CLA	C3A-C2A-CAA-CBA
24	B	604	CLA	C12-C13-C15-C16
24	B	611	CLA	C6-C7-C8-C10
24	C	503	CLA	C6-C7-C8-C10
24	C	506	CLA	C6-C7-C8-C10
24	C	511	CLA	C11-C12-C13-C15
24	C	513	CLA	C11-C10-C8-C7
24	b	604	CLA	C11-C12-C13-C15
24	b	605	CLA	C11-C12-C13-C15
24	b	605	CLA	C12-C13-C15-C16
24	b	607	CLA	C11-C12-C13-C15
24	c	505	CLA	C6-C7-C8-C10
24	c	509	CLA	C6-C7-C8-C10
24	c	512	CLA	C12-C13-C15-C16
27	d	407	PL9	C13-C14-C16-C17
33	l	101	LHG	O6-C4-C5-O7
26	b	620	BCR	C9-C10-C11-C12
28	a	411	SQD	C9-C10-C11-C12
29	c	518	DGD	C8B-C9B-CAB-CBB
32	M	101	LMG	C39-C40-C41-C42
33	l	101	LHG	C33-C34-C35-C36
24	C	503	CLA	O1A-CGA-O2A-C1
28	A	411	SQD	C33-C34-C35-C36
24	B	612	CLA	C16-C17-C18-C20
29	A	413	DGD	CCA-CDA-CEA-CFA
29	H	102	DGD	O1A-C1A-O1G-C1G
29	C	517	DGD	O1B-C1B-O2G-C2G
24	c	503	CLA	CBD-CGD-O2D-CED
28	b	601	SQD	O47-C45-C46-O48
28	f	101	SQD	O47-C45-C46-O48
29	C	516	DGD	O1G-C1G-C2G-O2G
33	D	409	LHG	C15-C16-C17-C18
33	L	101	LHG	C24-C25-C26-C27
24	B	601	CLA	C4-C3-C5-C6
24	B	612	CLA	CBA-CGA-O2A-C1
24	b	608	CLA	CBA-CGA-O2A-C1
32	c	524	LMG	C13-C14-C15-C16
24	B	611	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
24	B	616	CLA	C6-C7-C8-C9
24	C	505	CLA	C11-C10-C8-C9
24	C	509	CLA	C6-C7-C8-C9
24	C	511	CLA	C11-C12-C13-C14
24	C	512	CLA	C6-C7-C8-C9
24	D	404	CLA	C14-C13-C15-C16
24	b	603	CLA	C11-C10-C8-C9
24	b	605	CLA	C14-C13-C15-C16
24	b	608	CLA	C11-C12-C13-C14
24	c	505	CLA	C6-C7-C8-C9
24	c	509	CLA	C14-C13-C15-C16
26	b	618	BCR	C6-C7-C8-C9
33	d	409	LHG	O9-C7-O7-C5
28	B	622	SQD	C28-C29-C30-C31
24	h	101	CLA	C3-C5-C6-C7
24	d	405	CLA	C16-C17-C18-C19
32	K	102	LMG	C14-C15-C16-C17
29	C	516	DGD	CCA-CDA-CEA-CFA
24	B	604	CLA	C2C-C3C-CAC-CBC
29	H	102	DGD	CAB-CBB-CCB-CDB
33	d	408	LHG	C9-C10-C11-C12
29	C	517	DGD	CCB-CDB-CEB-CFB
33	l	101	LHG	C12-C13-C14-C15
24	c	512	CLA	C4-C3-C5-C6
29	h	104	DGD	O2G-C1B-C2B-C3B
24	C	505	CLA	C2-C3-C5-C6
24	B	603	CLA	C5-C6-C7-C8
24	D	403	CLA	C4C-C3C-CAC-CBC
29	c	517	DGD	C8A-C9A-CAA-CBA
32	D	410	LMG	C31-C32-C33-C34
28	a	411	SQD	C11-C10-C9-C8
32	b	621	LMG	C15-C16-C17-C18
32	D	407	LMG	C38-C39-C40-C41
33	D	408	LHG	C13-C14-C15-C16
33	L	101	LHG	C10-C11-C12-C13
28	f	101	SQD	C46-C45-O47-C7
29	a	412	DGD	C1G-C2G-O2G-C1B
32	b	623	LMG	C9-C8-O7-C10
24	B	603	CLA	C2A-CAA-CBA-CGA
33	D	411	LHG	C7-C8-C9-C10
28	b	601	SQD	C30-C31-C32-C33
29	c	518	DGD	CBB-CCB-CDB-CEB

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Mol	Chain	Res	Type	Atoms
29	a	412	DGD	O2G-C1B-C2B-C3B
33	D	408	LHG	C18-C19-C20-C21
33	D	409	LHG	C2-C3-O3-P
29	c	516	DGD	C6B-C7B-C8B-C9B
32	b	623	LMG	C38-C39-C40-C41
32	c	524	LMG	C17-C18-C19-C20
33	d	409	LHG	C25-C26-C27-C28
24	c	503	CLA	O1D-CGD-O2D-CED
28	b	601	SQD	C18-C19-C20-C21
24	C	514	CLA	C4-C3-C5-C6
28	A	412	SQD	C27-C28-C29-C30
26	B	619	BCR	C1-C6-C7-C8
26	b	618	BCR	C1-C6-C7-C8
26	c	521	BCR	C23-C24-C25-C30
26	k	101	BCR	C5-C6-C7-C8
29	a	412	DGD	CEB-CFB-CGB-CHB
32	c	524	LMG	C34-C35-C36-C37
29	A	413	DGD	O6E-C1E-O5D-C6D
28	b	601	SQD	C26-C27-C28-C29
25	A	407	PHO	C15-C16-C17-C18
26	B	617	BCR	C20-C21-C22-C23
26	c	514	BCR	C12-C13-C14-C15
29	A	413	DGD	C2E-C1E-O5D-C6D
29	c	516	DGD	O1G-C1G-C2G-O2G
28	a	411	SQD	C17-C18-C19-C20
33	d	409	LHG	C32-C33-C34-C35
29	A	413	DGD	C6B-C7B-C8B-C9B
27	A	410	PL9	C17-C18-C19-C21
32	b	621	LMG	C33-C34-C35-C36
24	C	506	CLA	C4-C3-C5-C6
29	c	516	DGD	CBB-CCB-CDB-CEB
24	C	507	CLA	C6-C7-C8-C10
29	c	516	DGD	C8A-C9A-CAA-CBA
24	B	612	CLA	C11-C10-C8-C9
24	B	613	CLA	C6-C7-C8-C9
24	b	609	CLA	C11-C10-C8-C9
24	c	501	CLA	C11-C12-C13-C14
26	b	618	BCR	C15-C16-C17-C18
24	a	405	CLA	C16-C17-C18-C19
33	l	101	LHG	C10-C11-C12-C13
32	c	522	LMG	C29-C30-C31-C32
24	c	503	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
24	D	403	CLA	C15-C16-C17-C18
24	b	612	CLA	C15-C16-C17-C18
32	C	501	LMG	C17-C18-C19-C20
33	D	411	LHG	C24-C25-C26-C27
26	C	515	BCR	C21-C22-C23-C24
32	c	522	LMG	C16-C17-C18-C19
33	e	101	LHG	O9-C7-O7-C5
24	b	604	CLA	C13-C15-C16-C17
27	a	409	PL9	C28-C29-C31-C32
29	C	518	DGD	C8B-C9B-CAB-CBB
32	M	101	LMG	C17-C18-C19-C20
32	b	621	LMG	C39-C40-C41-C42
24	b	615	CLA	C13-C15-C16-C17
28	a	410	SQD	C16-C17-C18-C19
34	e	102	HEM	CAD-CBD-CGD-O1D
26	t	101	BCR	C13-C14-C15-C16
24	B	613	CLA	C4-C3-C5-C6
33	d	408	LHG	C24-C25-C26-C27
24	a	407	CLA	O1A-CGA-O2A-C1
25	A	407	PHO	O1A-CGA-O2A-C1
28	A	411	SQD	C10-C11-C12-C13
33	d	408	LHG	C18-C19-C20-C21
33	L	101	LHG	C17-C18-C19-C20
32	D	407	LMG	C17-C18-C19-C20
24	B	607	CLA	C3A-C2A-CAA-CBA
24	C	507	CLA	C3A-C2A-CAA-CBA
35	V	201	HEC	CAD-CBD-CGD-O2D
28	A	412	SQD	C44-C45-O47-C7
32	b	621	LMG	C22-C23-C24-C25
24	c	513	CLA	CBA-CGA-O2A-C1
25	D	401	PHO	C5-C6-C7-C8
24	B	609	CLA	C4-C3-C5-C6
29	H	102	DGD	C7B-C8B-C9B-CAB
27	A	410	PL9	C4-C3-C7-C8
24	C	510	CLA	C11-C10-C8-C9
24	b	605	CLA	C6-C7-C8-C9
24	b	612	CLA	C16-C17-C18-C20
28	a	411	SQD	C25-C26-C27-C28
32	c	524	LMG	C29-C30-C31-C32
26	B	619	BCR	C35-C13-C14-C15
26	b	602	BCR	C16-C17-C18-C36
29	c	516	DGD	O1G-C1G-C2G-C3G

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Mol	Chain	Res	Type	Atoms
34	F	102	HEM	CAD-CBD-CGD-O1D
24	B	603	CLA	C8-C10-C11-C12
24	B	612	CLA	O1A-CGA-O2A-C1
24	D	404	CLA	O2A-C1-C2-C3
25	a	406	PHO	O2A-C1-C2-C3
24	d	405	CLA	O1D-CGD-O2D-CED
29	C	516	DGD	O6E-C1E-O5D-C6D
26	b	602	BCR	C36-C18-C19-C20
35	V	201	HEC	CAD-CBD-CGD-O1D
28	a	410	SQD	C27-C28-C29-C30
32	D	407	LMG	C16-C17-C18-C19
28	f	101	SQD	C44-C45-O47-C7
32	C	501	LMG	C7-C8-O7-C10
24	B	602	CLA	C1A-C2A-CAA-CBA
24	c	508	CLA	C1A-C2A-CAA-CBA
24	A	406	CLA	C11-C12-C13-C15
24	B	601	CLA	C2-C3-C5-C6
24	B	603	CLA	C12-C13-C15-C16
24	B	613	CLA	C6-C7-C8-C10
24	C	510	CLA	C12-C13-C15-C16
24	C	511	CLA	C12-C13-C15-C16
24	b	606	CLA	C11-C10-C8-C7
24	b	607	CLA	C12-C13-C15-C16
24	c	503	CLA	C11-C10-C8-C7
24	c	506	CLA	C6-C7-C8-C10
24	c	513	CLA	C12-C13-C15-C16
24	d	404	CLA	C11-C12-C13-C15
29	H	102	DGD	C2B-C3B-C4B-C5B
26	k	101	BCR	C13-C14-C15-C16
32	M	101	LMG	C35-C36-C37-C38
33	e	101	LHG	C25-C26-C27-C28
24	C	508	CLA	O1D-CGD-O2D-CED
34	e	102	HEM	CAD-CBD-CGD-O2D
35	v	201	HEC	CAD-CBD-CGD-O2D
28	f	101	SQD	C34-C35-C36-C37
29	c	516	DGD	C7B-C8B-C9B-CAB
32	b	621	LMG	O6-C5-C6-O5
28	b	601	SQD	C25-C26-C27-C28
24	B	610	CLA	C15-C16-C17-C18
33	D	409	LHG	O6-C4-C5-C6
27	A	410	PL9	C32-C33-C34-C35
24	C	505	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
24	B	615	CLA	C5-C6-C7-C8
32	c	522	LMG	C28-C29-C30-C31
35	v	201	HEC	CAD-CBD-CGD-O1D
33	e	101	LHG	C18-C19-C20-C21
24	B	613	CLA	C13-C15-C16-C17
26	c	521	BCR	C20-C21-C22-C23
24	c	505	CLA	O1D-CGD-O2D-CED
24	c	511	CLA	C3-C5-C6-C7
26	d	406	BCR	C22-C23-C24-C25
29	c	518	DGD	C2A-C3A-C4A-C5A
32	c	524	LMG	C19-C20-C21-C22
27	A	410	PL9	C34-C36-C37-C38
27	A	410	PL9	C39-C41-C42-C43
32	D	410	LMG	O1-C7-C8-C9
24	B	603	CLA	C4-C3-C5-C6
24	c	508	CLA	C4-C3-C5-C6
24	A	408	CLA	C5-C6-C7-C8
32	b	621	LMG	C14-C15-C16-C17
24	D	403	CLA	C2-C1-O2A-CGA
24	B	609	CLA	C2-C3-C5-C6
24	C	506	CLA	C2-C3-C5-C6
33	D	409	LHG	C13-C14-C15-C16
29	H	102	DGD	CAA-CBA-CCA-CDA
24	C	512	CLA	C11-C10-C8-C9
24	c	513	CLA	O1A-CGA-O2A-C1
24	c	513	CLA	C3-C5-C6-C7
33	L	101	LHG	C14-C15-C16-C17
28	a	411	SQD	C24-C25-C26-C27
26	A	409	BCR	C23-C24-C25-C26
26	A	409	BCR	C23-C24-C25-C30
26	B	618	BCR	C23-C24-C25-C26
26	B	618	BCR	C23-C24-C25-C30
26	t	101	BCR	C5-C6-C7-C8
24	c	509	CLA	CAA-CBA-CGA-O2A
29	c	516	DGD	O1G-C1A-C2A-C3A
34	F	102	HEM	CAD-CBD-CGD-O2D
24	C	504	CLA	C8-C10-C11-C12
24	b	603	CLA	C13-C15-C16-C17
24	b	605	CLA	C8-C10-C11-C12
26	c	521	BCR	C15-C16-C17-C18
26	c	521	BCR	C17-C18-C19-C20
29	a	412	DGD	C9A-CAA-CBA-CCA

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Mol	Chain	Res	Type	Atoms
24	c	505	CLA	C2-C3-C5-C6
24	c	512	CLA	C2-C3-C5-C6
24	b	603	CLA	C8-C10-C11-C12
28	A	411	SQD	C12-C13-C14-C15
29	c	516	DGD	C1B-C2B-C3B-C4B
32	B	621	LMG	C37-C38-C39-C40
32	c	522	LMG	C35-C36-C37-C38
24	c	509	CLA	C3-C5-C6-C7
24	B	608	CLA	C16-C17-C18-C20
32	c	519	LMG	C32-C33-C34-C35
33	e	101	LHG	O6-C4-C5-C6
29	C	516	DGD	CBA-CCA-CDA-CEA
29	c	516	DGD	CBA-CCA-CDA-CEA
24	B	612	CLA	C11-C10-C8-C7
24	D	403	CLA	C12-C13-C15-C16
33	D	411	LHG	O1-C1-C2-O2
32	D	410	LMG	O1-C7-C8-O7
32	b	623	LMG	C40-C41-C42-C43
33	L	101	LHG	O9-C7-O7-C5
25	A	407	PHO	CBA-CGA-O2A-C1
29	c	518	DGD	C9A-CAA-CBA-CCA
24	b	613	CLA	CAA-CBA-CGA-O2A
28	a	410	SQD	O47-C7-C8-C9
33	D	409	LHG	C16-C17-C18-C19
25	d	402	PHO	C4C-C3C-CAC-CBC
27	d	407	PL9	C45-C44-C46-C47
29	c	517	DGD	C3A-C4A-C5A-C6A
27	A	410	PL9	C13-C14-C16-C17
24	B	612	CLA	CAA-CBA-CGA-O2A
24	B	603	CLA	C6-C7-C8-C9
24	B	604	CLA	C14-C13-C15-C16
24	B	605	CLA	C14-C13-C15-C16
24	C	503	CLA	C14-C13-C15-C16
24	C	506	CLA	C6-C7-C8-C9
24	C	511	CLA	C14-C13-C15-C16
24	b	605	CLA	C11-C12-C13-C14
24	b	607	CLA	C11-C12-C13-C14
24	c	503	CLA	C11-C10-C8-C9
24	c	512	CLA	C14-C13-C15-C16
24	c	513	CLA	C14-C13-C15-C16
25	a	406	PHO	C14-C13-C15-C16
29	c	517	DGD	C9A-CAA-CBA-CCA

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Mol	Chain	Res	Type	Atoms
33	l	101	LHG	C30-C31-C32-C33
28	a	411	SQD	C30-C31-C32-C33
29	h	104	DGD	C5A-C6A-C7A-C8A
24	B	605	CLA	CAD-CBD-CGD-O2D
24	B	610	CLA	CAD-CBD-CGD-O2D
24	C	504	CLA	CAD-CBD-CGD-O2D
24	C	507	CLA	CAD-CBD-CGD-O2D
24	C	513	CLA	CAD-CBD-CGD-O2D
24	b	604	CLA	CAD-CBD-CGD-O2D
24	b	605	CLA	CAD-CBD-CGD-O2D
24	b	611	CLA	CAD-CBD-CGD-O2D
28	a	411	SQD	C26-C27-C28-C29
28	b	601	SQD	C15-C16-C17-C18
24	B	613	CLA	C2-C1-O2A-CGA
28	A	411	SQD	O47-C7-C8-C9
26	k	101	BCR	C22-C23-C24-C25
24	B	616	CLA	O1A-CGA-O2A-C1
24	D	404	CLA	C13-C15-C16-C17
33	E	101	LHG	C10-C11-C12-C13
24	A	405	CLA	C13-C15-C16-C17
27	A	410	PL9	C28-C29-C31-C32
27	D	406	PL9	C43-C44-C46-C47
32	C	501	LMG	C34-C35-C36-C37
26	B	618	BCR	C11-C12-C13-C14
26	H	101	BCR	C21-C22-C23-C24
33	D	411	LHG	C16-C17-C18-C19
33	e	101	LHG	C10-C11-C12-C13
25	D	401	PHO	C2C-C3C-CAC-CBC
25	d	402	PHO	C2C-C3C-CAC-CBC
29	h	104	DGD	CAA-CBA-CCA-CDA
32	h	102	LMG	O9-C10-C11-C12
32	M	101	LMG	C11-C12-C13-C14
33	d	410	LHG	C24-C23-O8-C6
24	b	603	CLA	C2A-CAA-CBA-CGA
29	a	412	DGD	CDB-CEB-CFB-CGB
33	d	409	LHG	C12-C13-C14-C15
28	a	410	SQD	C24-C25-C26-C27
28	a	410	SQD	C19-C20-C21-C22
33	d	408	LHG	C27-C28-C29-C30
24	A	406	CLA	CHA-CBD-CGD-O2D
24	B	602	CLA	CHA-CBD-CGD-O1D
24	B	602	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
24	B	606	CLA	CHA-CBD-CGD-O2D
24	B	607	CLA	CHA-CBD-CGD-O1D
24	B	612	CLA	CHA-CBD-CGD-O1D
24	B	612	CLA	CHA-CBD-CGD-O2D
24	C	504	CLA	CHA-CBD-CGD-O2D
24	C	508	CLA	CHA-CBD-CGD-O1D
24	C	508	CLA	CHA-CBD-CGD-O2D
24	C	510	CLA	CHA-CBD-CGD-O1D
24	C	510	CLA	CHA-CBD-CGD-O2D
24	a	405	CLA	CHA-CBD-CGD-O1D
24	a	405	CLA	CHA-CBD-CGD-O2D
24	b	604	CLA	CHA-CBD-CGD-O2D
24	b	607	CLA	CHA-CBD-CGD-O2D
24	b	610	CLA	CHA-CBD-CGD-O1D
24	c	510	CLA	CHA-CBD-CGD-O2D
26	t	101	BCR	C9-C10-C11-C12
33	D	409	LHG	C32-C33-C34-C35
26	c	521	BCR	C12-C13-C14-C15
24	B	613	CLA	CAA-CBA-CGA-O2A
24	c	510	CLA	CAA-CBA-CGA-O2A
32	C	501	LMG	O1-C7-C8-O7
24	B	607	CLA	C5-C6-C7-C8
29	C	518	DGD	CBB-CCB-CDB-CEB
32	c	524	LMG	O8-C28-C29-C30
24	c	501	CLA	C2A-CAA-CBA-CGA
25	d	402	PHO	CHA-CBD-CGD-O1D
25	d	402	PHO	CHA-CBD-CGD-O2D
24	A	406	CLA	C15-C16-C17-C18
32	b	621	LMG	C40-C41-C42-C43
32	b	623	LMG	C32-C33-C34-C35
33	D	408	LHG	C16-C17-C18-C19
29	c	516	DGD	C3B-C4B-C5B-C6B
29	c	517	DGD	CCA-CDA-CEA-CFA
24	B	605	CLA	C12-C13-C15-C16
24	C	512	CLA	C6-C7-C8-C10
24	b	606	CLA	C12-C13-C15-C16
24	b	610	CLA	C11-C12-C13-C15
24	c	509	CLA	C11-C10-C8-C7
32	M	101	LMG	C30-C31-C32-C33
28	b	601	SQD	O47-C7-C8-C9
33	L	101	LHG	O7-C7-C8-C9
32	h	102	LMG	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
24	A	406	CLA	C11-C12-C13-C14
24	B	603	CLA	C14-C13-C15-C16
24	C	504	CLA	C6-C7-C8-C9
24	C	510	CLA	C14-C13-C15-C16
24	C	512	CLA	C11-C12-C13-C14
24	b	606	CLA	C14-C13-C15-C16
24	h	101	CLA	C11-C12-C13-C14
33	e	101	LHG	C19-C20-C21-C22
28	f	101	SQD	C29-C30-C31-C32
29	h	104	DGD	CBB-CCB-CDB-CEB
33	D	411	LHG	C24-C23-O8-C6
28	f	101	SQD	O48-C23-C24-C25
32	b	621	LMG	O9-C10-C11-C12
28	a	410	SQD	C25-C26-C27-C28
28	A	412	SQD	C8-C7-O47-C45
28	a	410	SQD	C8-C7-O47-C45
24	B	614	CLA	C2A-CAA-CBA-CGA
24	b	611	CLA	C2A-CAA-CBA-CGA
32	K	102	LMG	C18-C19-C20-C21
24	b	614	CLA	CAA-CBA-CGA-O2A
33	d	408	LHG	O8-C23-C24-C25
26	d	406	BCR	C7-C8-C9-C34
32	b	623	LMG	O7-C10-C11-C12
32	b	623	LMG	O9-C10-C11-C12
32	D	410	LMG	C16-C17-C18-C19
24	B	604	CLA	C1A-C2A-CAA-CBA
24	B	607	CLA	C1A-C2A-CAA-CBA
24	C	507	CLA	C1A-C2A-CAA-CBA
24	C	513	CLA	C1A-C2A-CAA-CBA
29	C	516	DGD	C6A-C7A-C8A-C9A
24	b	614	CLA	CAA-CBA-CGA-O1A
33	e	101	LHG	O10-C23-C24-C25
24	B	612	CLA	CAA-CBA-CGA-O1A
24	b	613	CLA	CAA-CBA-CGA-O1A
28	b	601	SQD	O6-C44-C45-C46
32	c	524	LMG	O1-C7-C8-C9
29	C	516	DGD	O2G-C1B-C2B-C3B
24	B	603	CLA	CBD-CGD-O2D-CED
32	C	501	LMG	C8-C9-O8-C28
27	d	407	PL9	C30-C29-C31-C32
33	L	101	LHG	C15-C16-C17-C18
24	C	514	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
28	A	411	SQD	C9-C10-C11-C12
29	H	102	DGD	C8B-C9B-CAB-CBB
32	B	621	LMG	O8-C28-C29-C30
29	C	516	DGD	C2E-C1E-O5D-C6D
24	c	512	CLA	C8-C10-C11-C12
29	c	517	DGD	CAA-CBA-CCA-CDA
33	D	408	LHG	C4-O6-P-O5
33	E	101	LHG	C4-O6-P-O5
33	L	101	LHG	C4-O6-P-O5
33	d	409	LHG	C4-O6-P-O5
24	c	510	CLA	CAA-CBA-CGA-O1A
28	A	411	SQD	C17-C18-C19-C20
26	t	101	BCR	C1-C6-C7-C8
28	A	411	SQD	C27-C28-C29-C30
24	C	514	CLA	C5-C6-C7-C8
32	D	407	LMG	C15-C16-C17-C18
32	K	102	LMG	C38-C39-C40-C41
24	b	615	CLA	C2A-CAA-CBA-CGA
29	c	516	DGD	O1B-C1B-C2B-C3B
24	c	506	CLA	C8-C10-C11-C12
33	e	101	LHG	C11-C10-C9-C8
33	D	409	LHG	O10-C23-C24-C25
24	c	504	CLA	C11-C12-C13-C15
24	B	607	CLA	CAD-CBD-CGD-O1D
24	B	611	CLA	CAD-CBD-CGD-O1D
24	B	612	CLA	CAD-CBD-CGD-O1D
24	b	608	CLA	CAD-CBD-CGD-O1D
24	b	610	CLA	CAD-CBD-CGD-O1D
24	c	506	CLA	CAD-CBD-CGD-O1D
24	c	510	CLA	CAD-CBD-CGD-O1D
24	d	403	CLA	CAD-CBD-CGD-O1D
32	C	501	LMG	C9-C8-O7-C10
33	D	409	LHG	C4-C5-O7-C7
29	c	516	DGD	O2G-C1B-C2B-C3B
24	C	506	CLA	C14-C13-C15-C16
24	C	512	CLA	C14-C13-C15-C16
24	b	608	CLA	C11-C10-C8-C9
24	c	506	CLA	C14-C13-C15-C16
24	d	403	CLA	C11-C12-C13-C14
24	d	404	CLA	C11-C12-C13-C14
32	c	522	LMG	C39-C40-C41-C42
24	b	611	CLA	C13-C15-C16-C17

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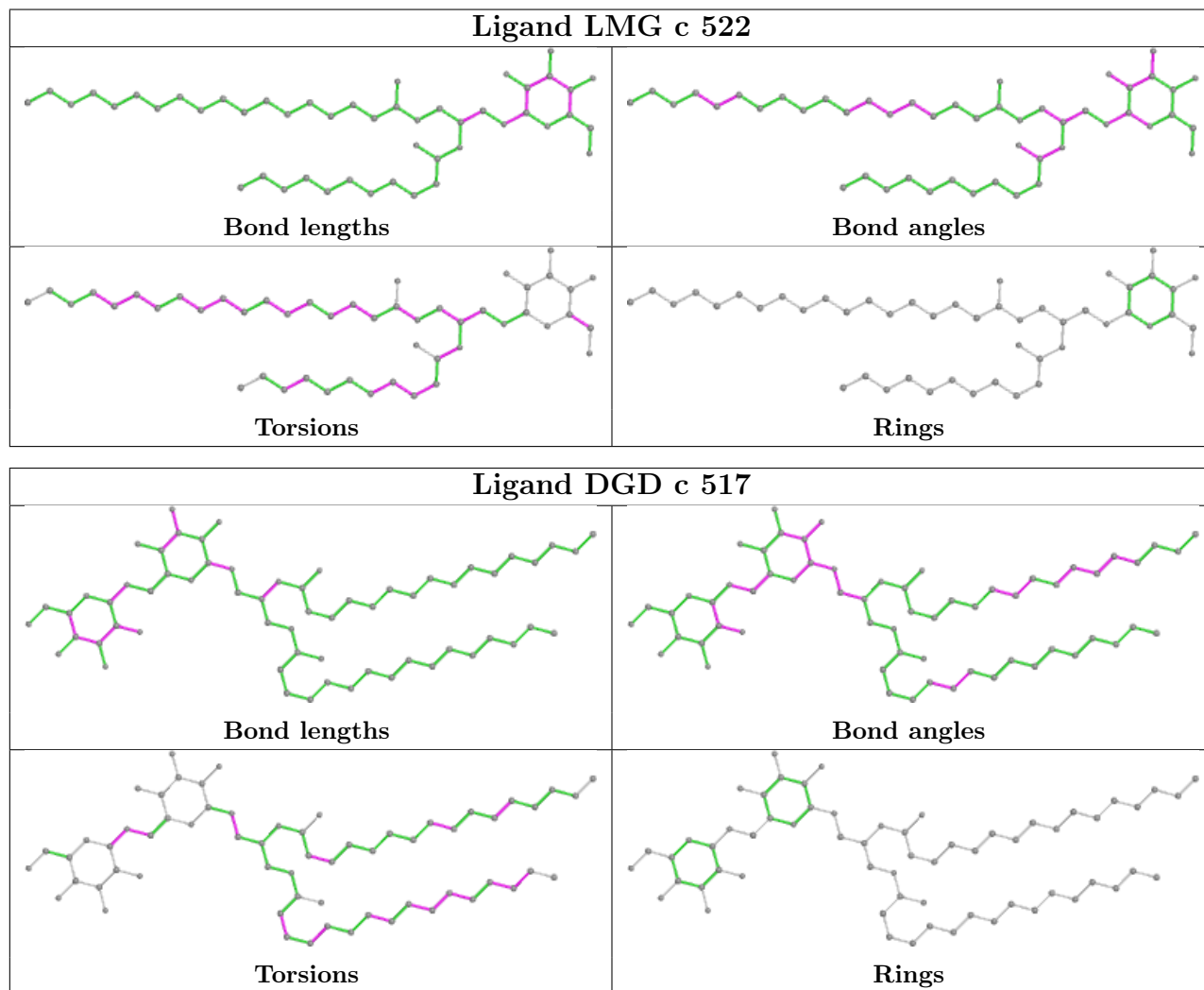
Mol	Chain	Res	Type	Atoms
28	F	101	SQD	C34-C35-C36-C37
24	B	613	CLA	CAA-CBA-CGA-O1A
24	a	407	CLA	CAA-CBA-CGA-O2A
33	l	101	LHG	O9-C7-O7-C5
24	B	604	CLA	C4-C3-C5-C6
24	c	505	CLA	C4-C3-C5-C6
24	B	607	CLA	C12-C13-C15-C16
24	C	503	CLA	C12-C13-C15-C16
24	C	512	CLA	C11-C12-C13-C15
24	b	611	CLA	C11-C12-C13-C15
24	b	614	CLA	C11-C12-C13-C15
24	c	506	CLA	C12-C13-C15-C16
24	c	512	CLA	C11-C10-C8-C7
24	h	101	CLA	C11-C10-C8-C7
34	e	102	HEM	CAA-CBA-CGA-O2A
29	c	518	DGD	O1G-C1A-C2A-C3A
32	b	621	LMG	O7-C10-C11-C12
33	D	411	LHG	C19-C20-C21-C22
24	c	507	CLA	C3-C5-C6-C7
26	H	101	BCR	C17-C18-C19-C20
26	c	514	BCR	C17-C18-C19-C20
24	B	608	CLA	C16-C17-C18-C19
28	B	622	SQD	O48-C23-C24-C25
28	a	410	SQD	O48-C23-C24-C25
24	d	403	CLA	C4C-C3C-CAC-CBC
29	C	517	DGD	O6D-C1D-O3G-C3G
29	C	517	DGD	CAA-CBA-CCA-CDA
28	a	410	SQD	O49-C7-C8-C9
29	c	518	DGD	O1B-C1B-C2B-C3B
32	C	501	LMG	O10-C28-C29-C30
28	A	412	SQD	C19-C20-C21-C22
24	c	504	CLA	C8-C10-C11-C12
29	C	518	DGD	CCB-CDB-CEB-CFB
24	b	611	CLA	C4C-C3C-CAC-CBC
24	C	503	CLA	C15-C16-C17-C18
24	b	613	CLA	C3-C5-C6-C7
24	b	617	CLA	C4-C3-C5-C6

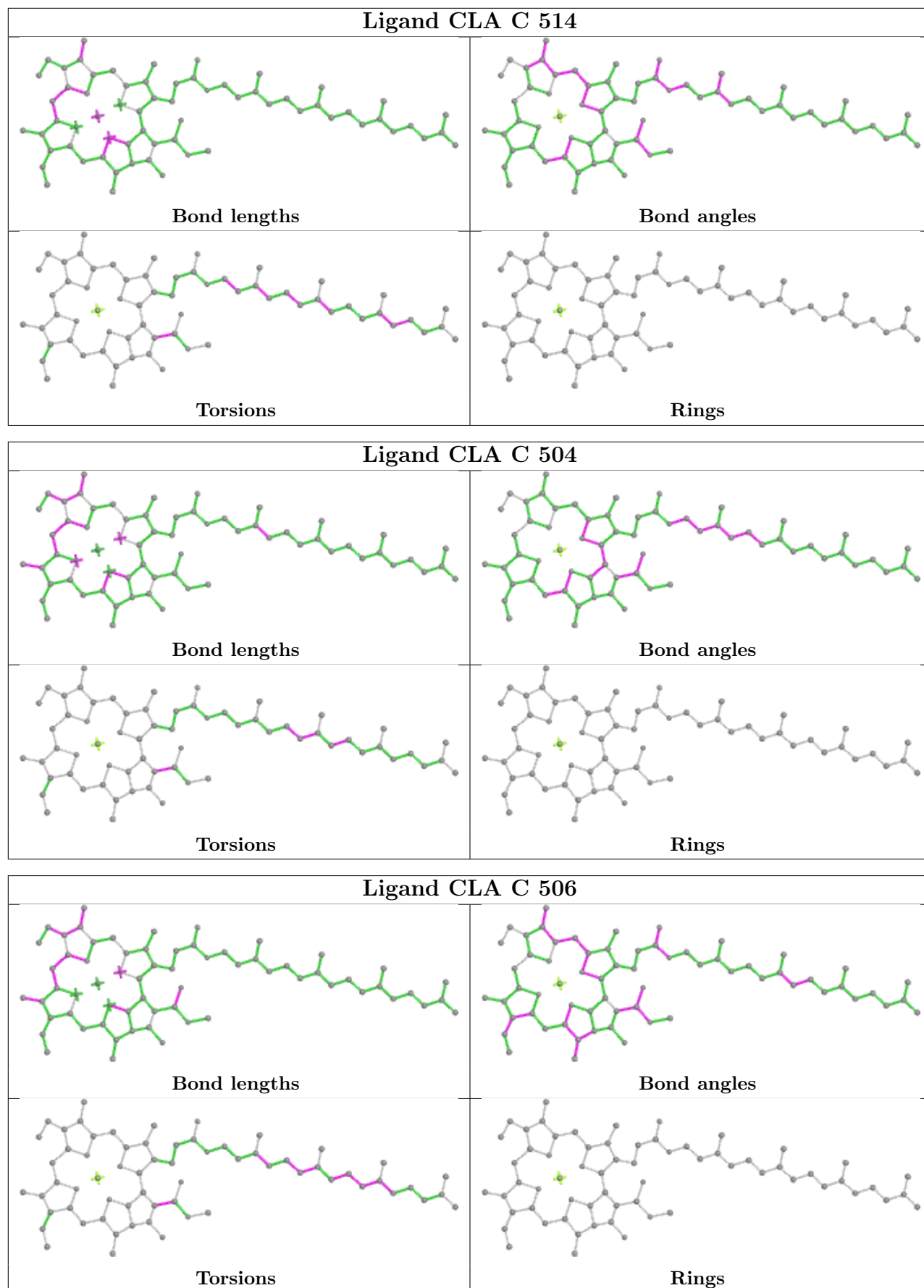
There are no ring outliers.

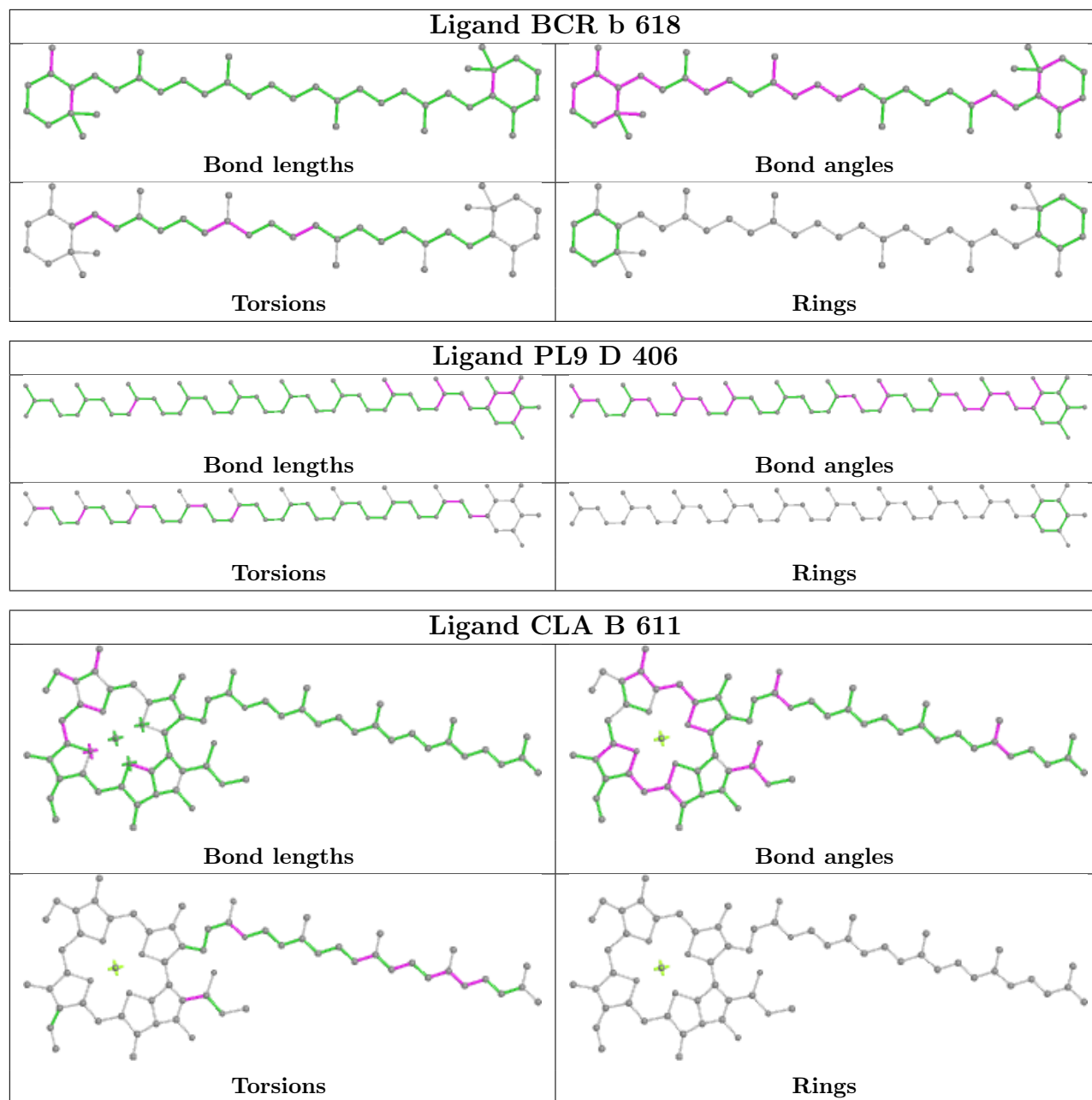
No monomer is involved in short contacts.

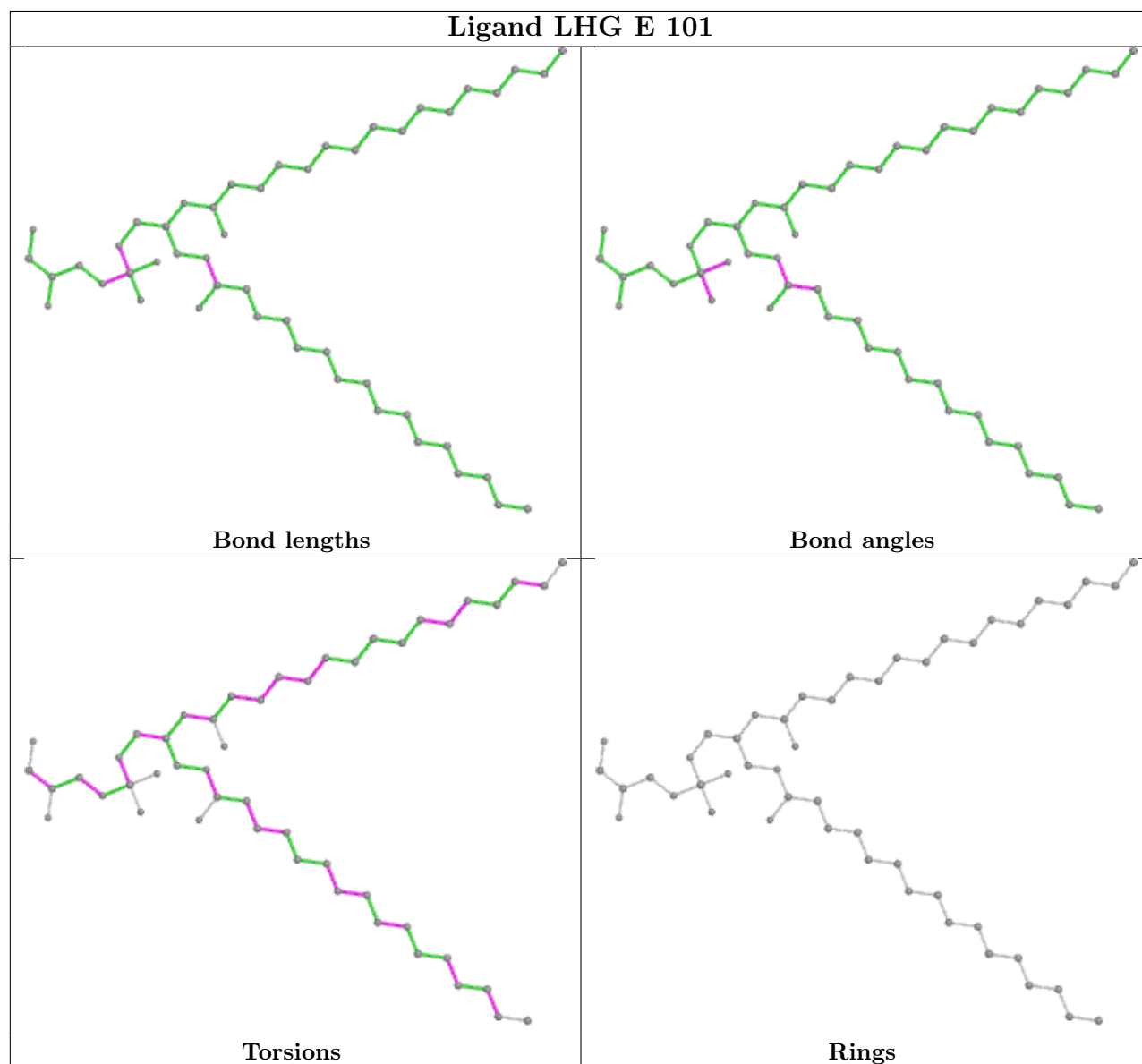
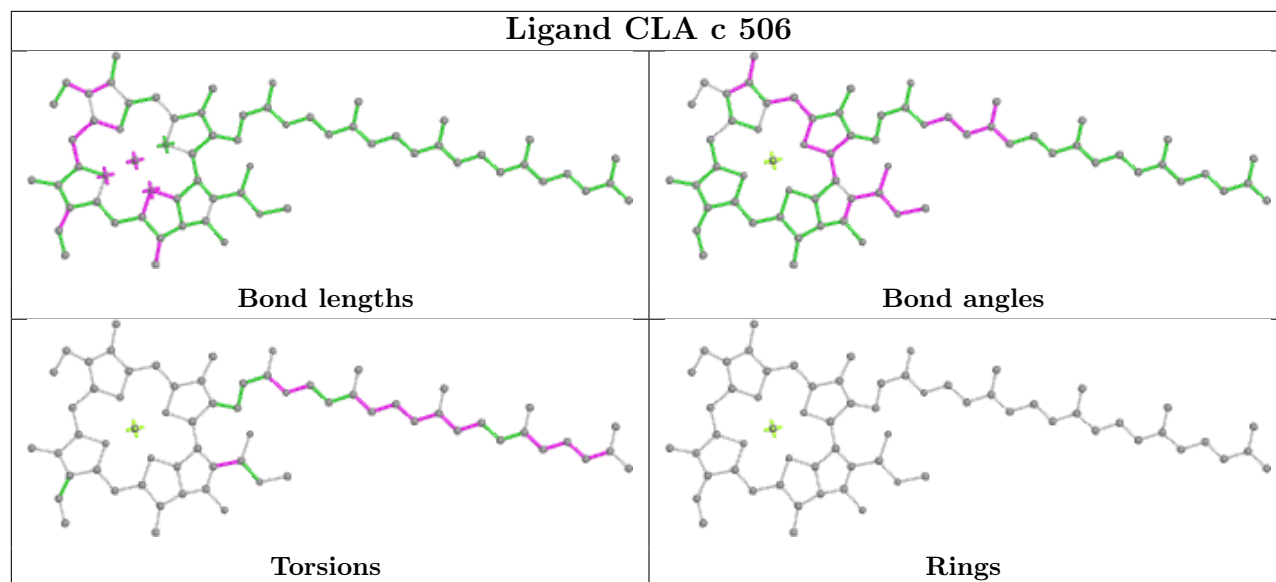
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

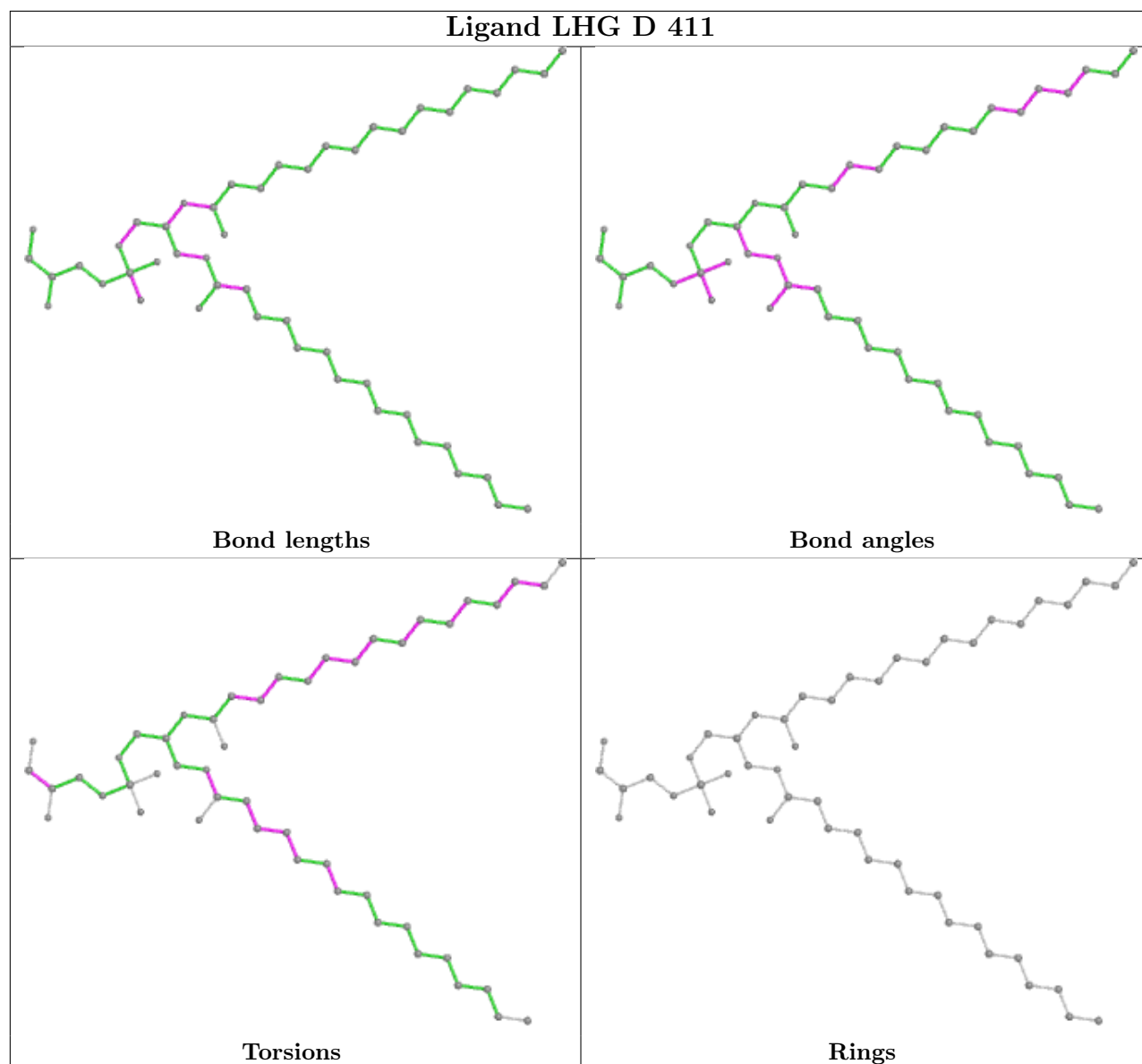
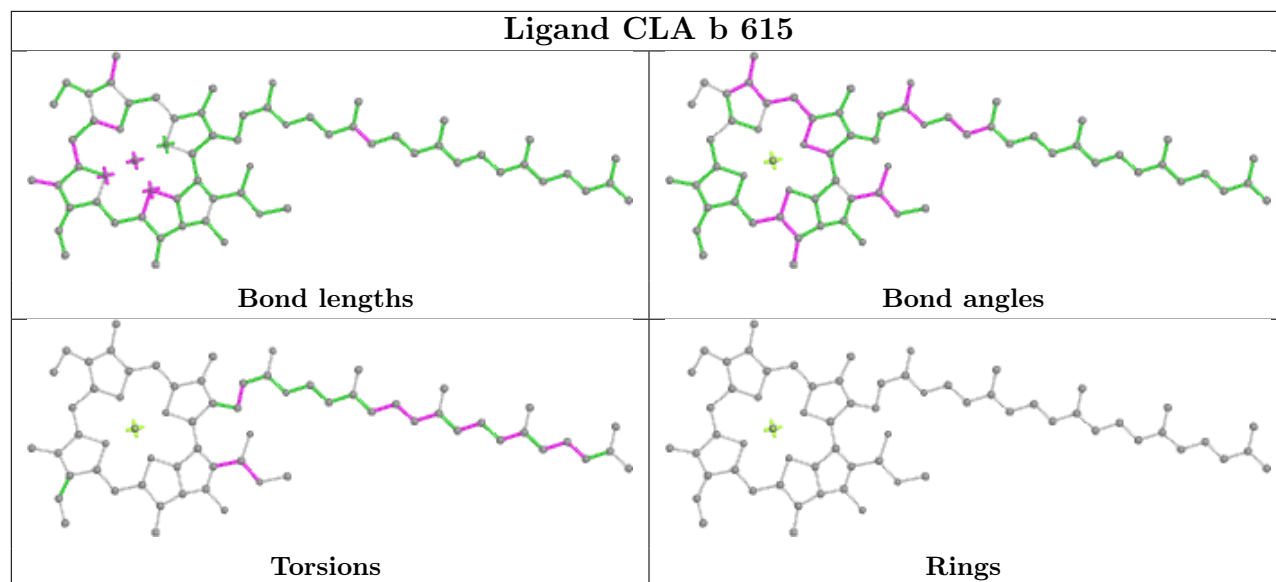
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

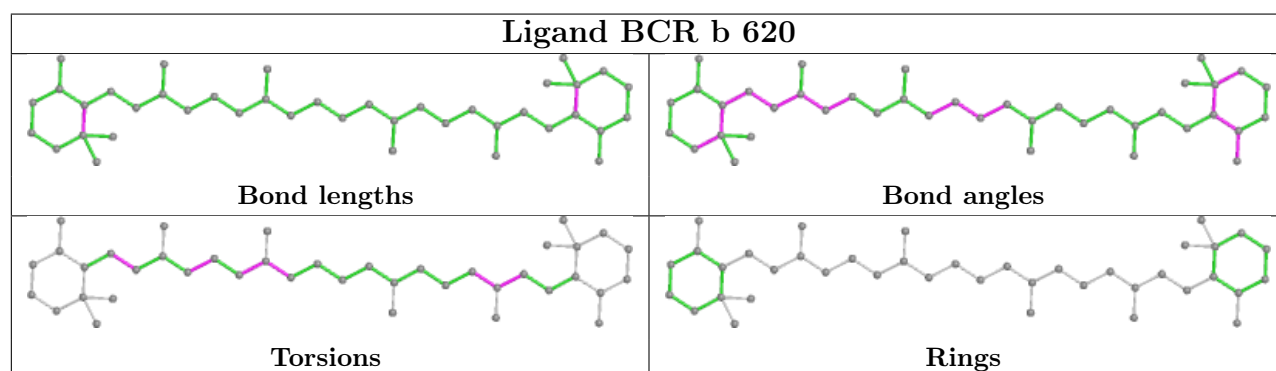
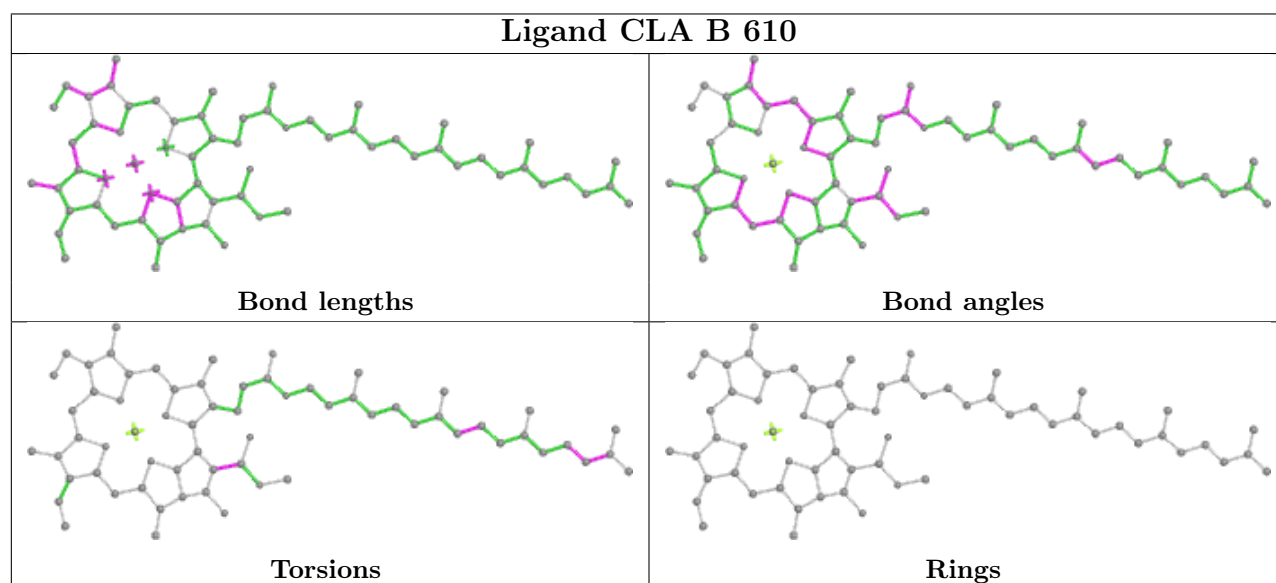
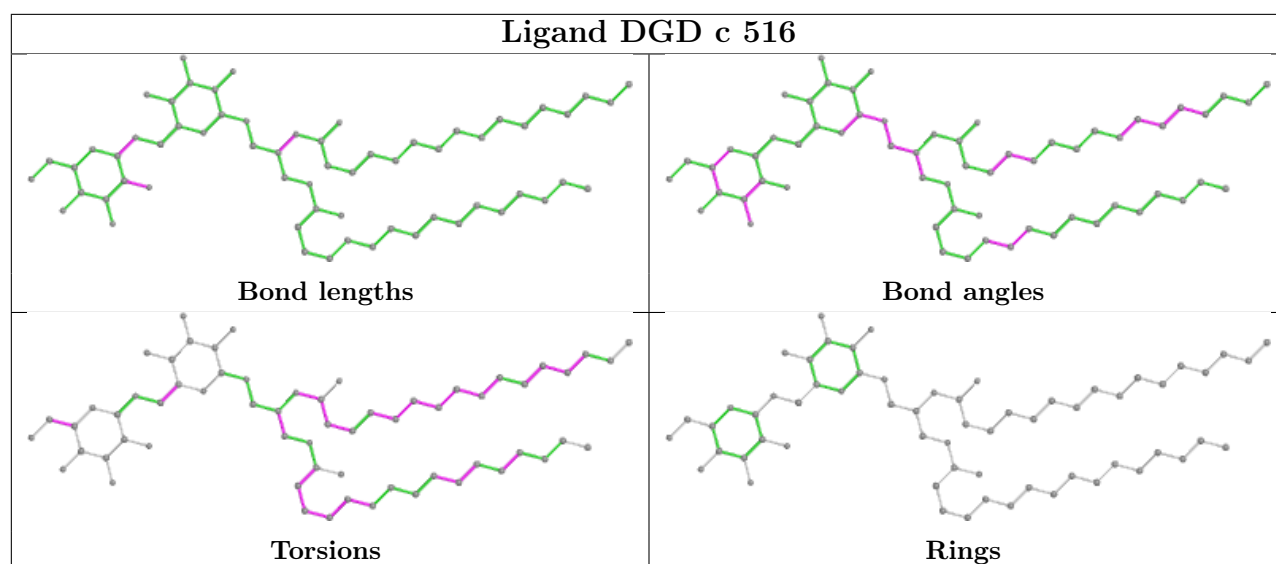


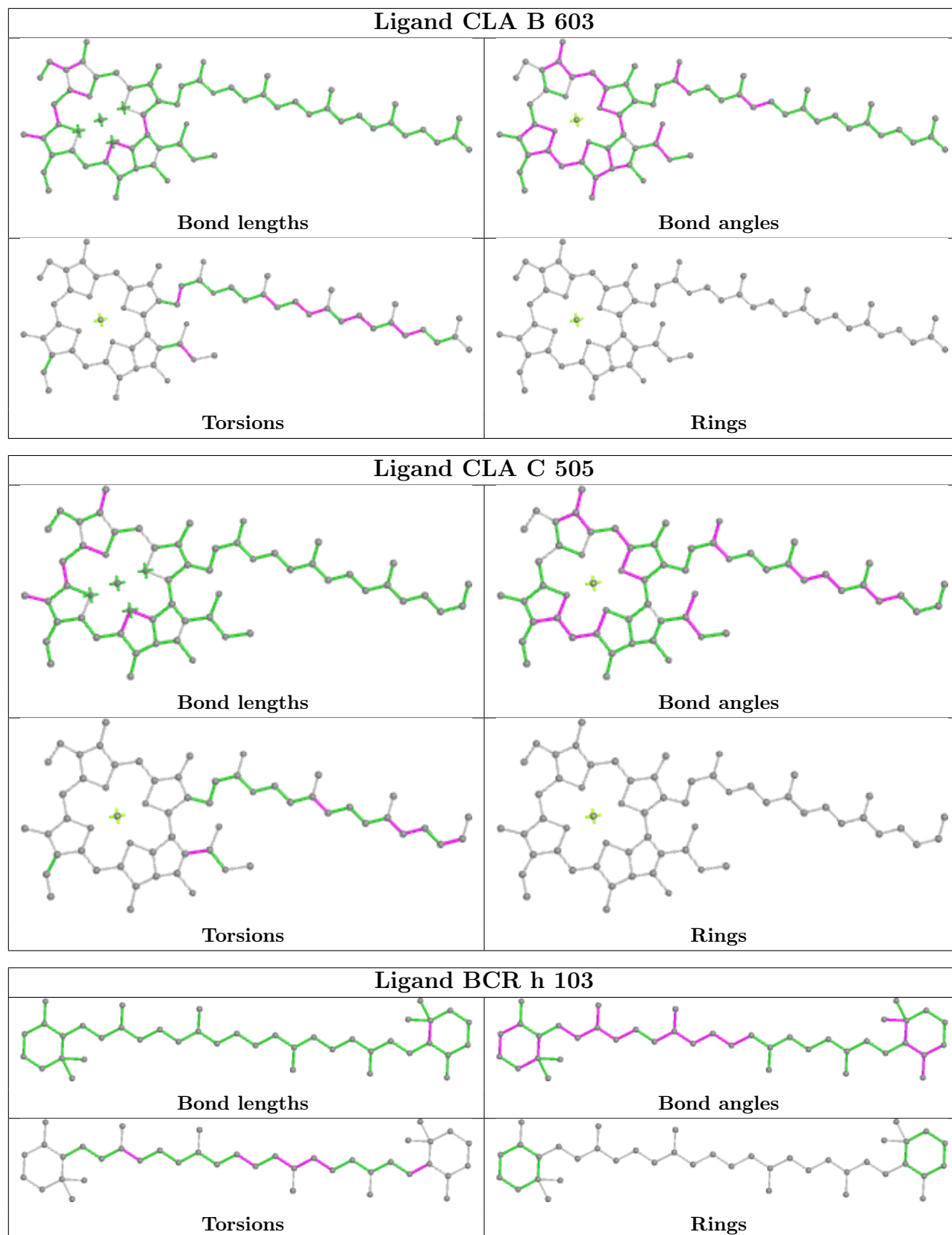


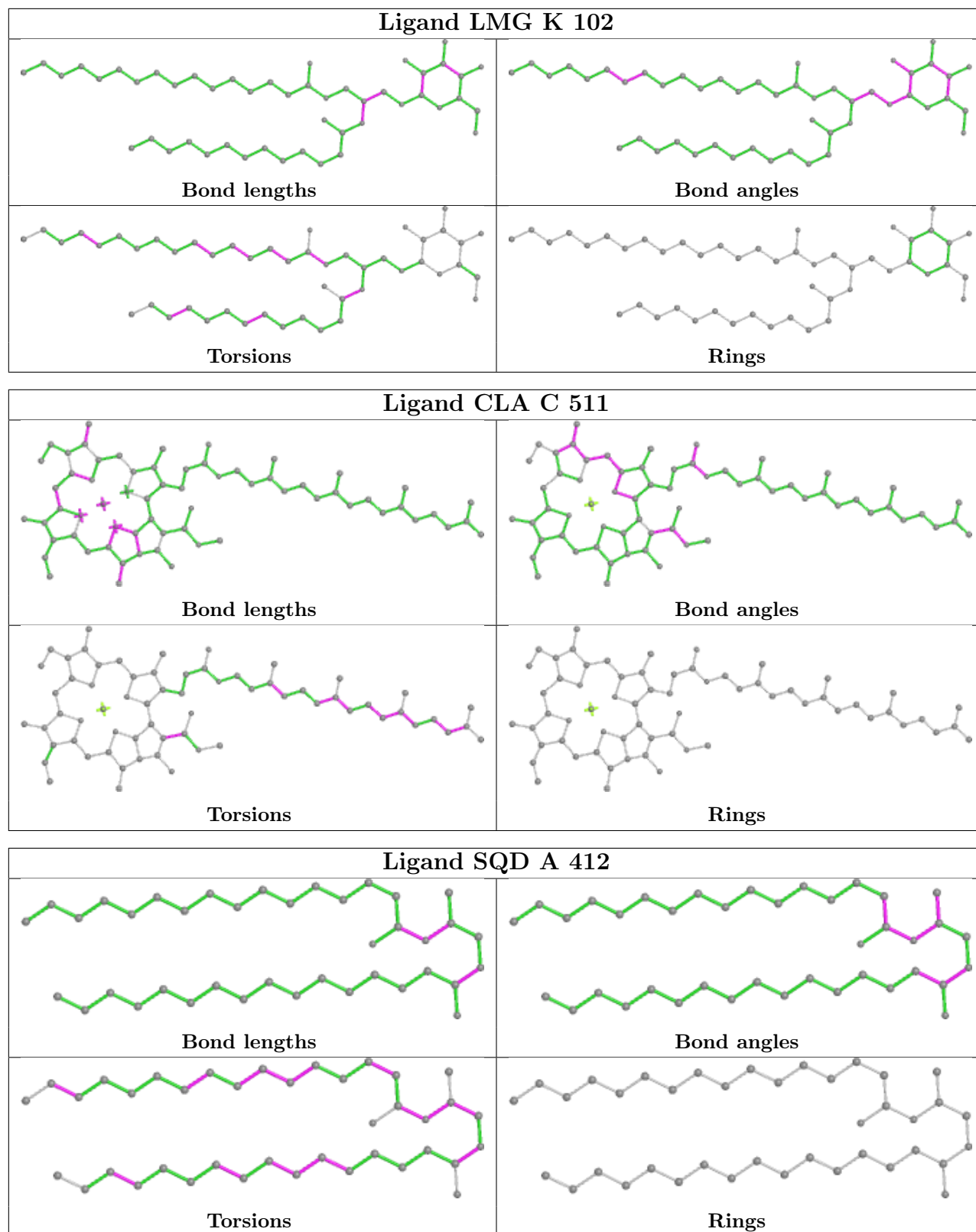


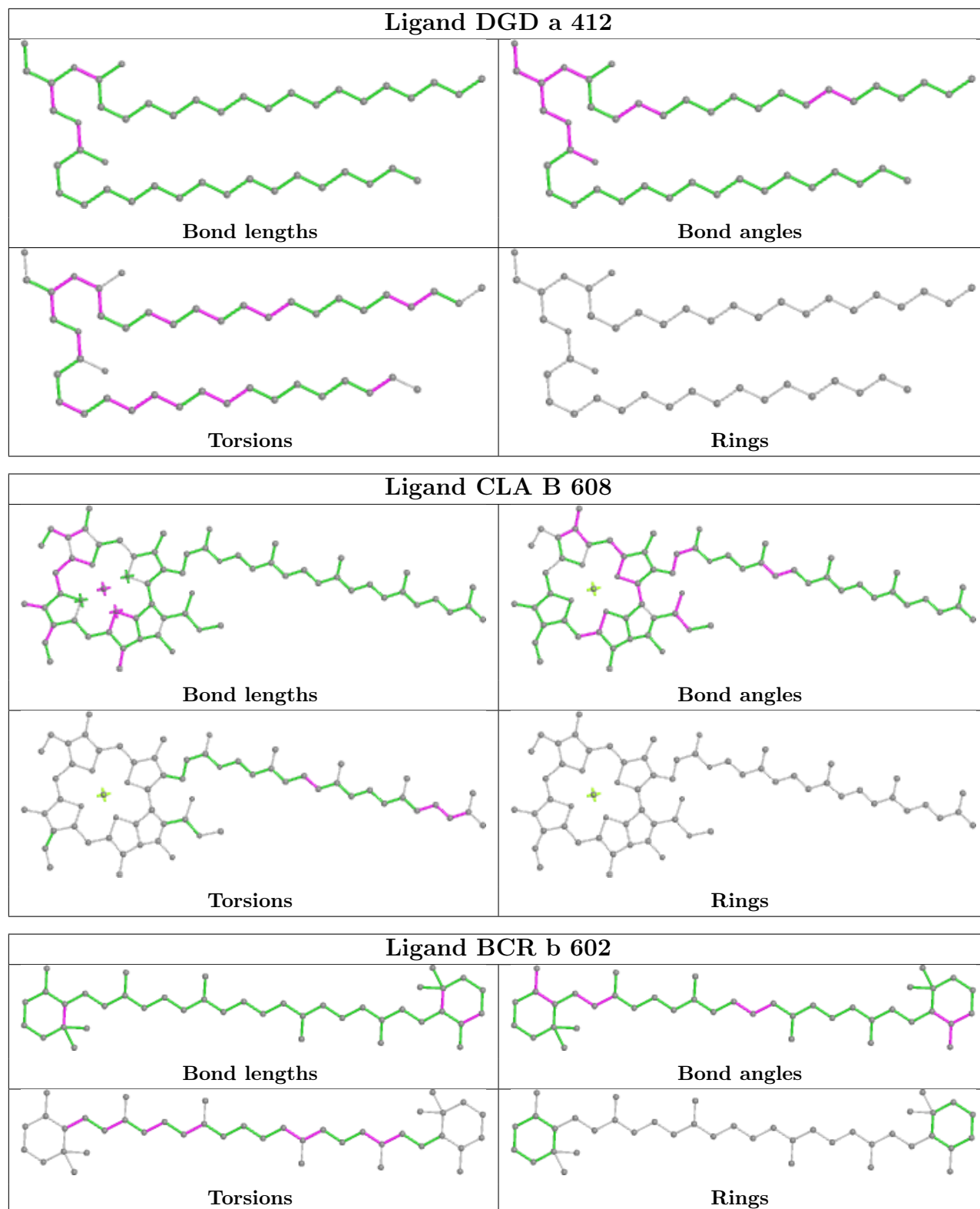


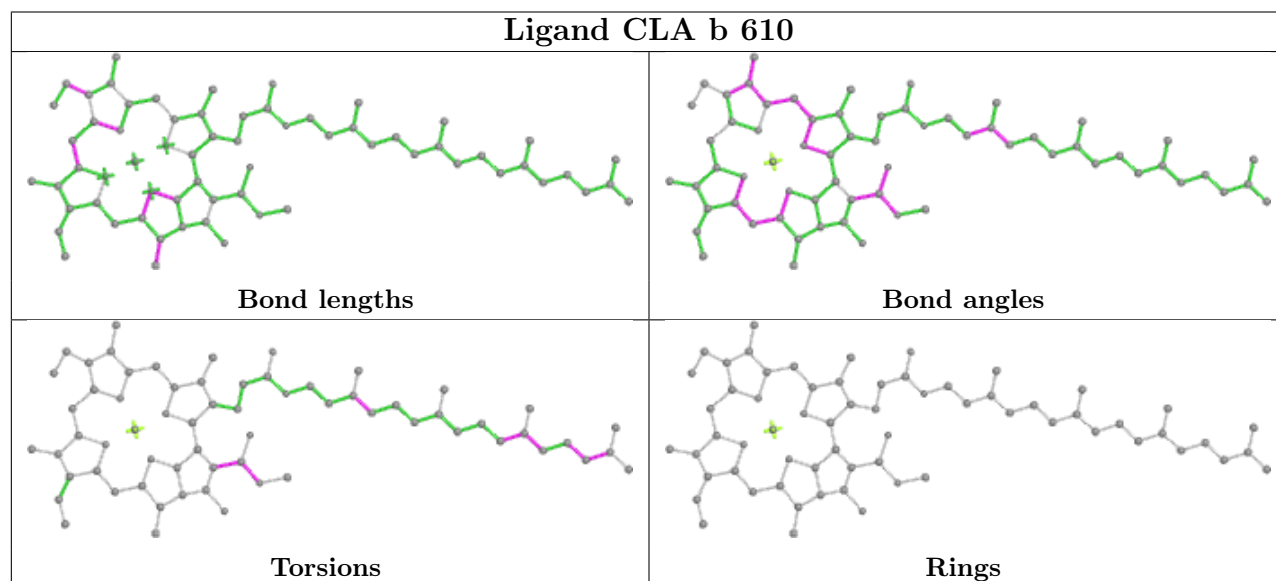
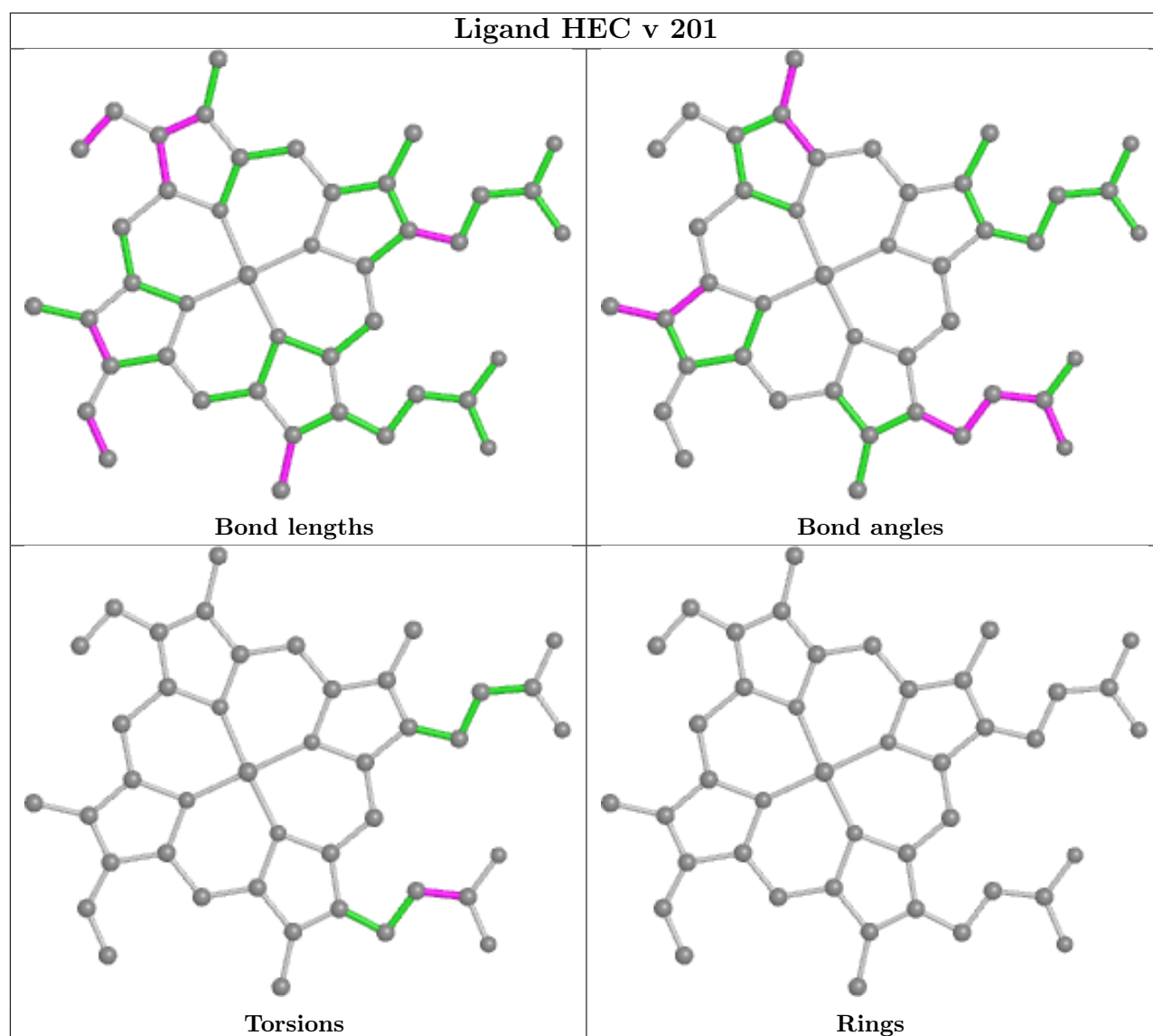


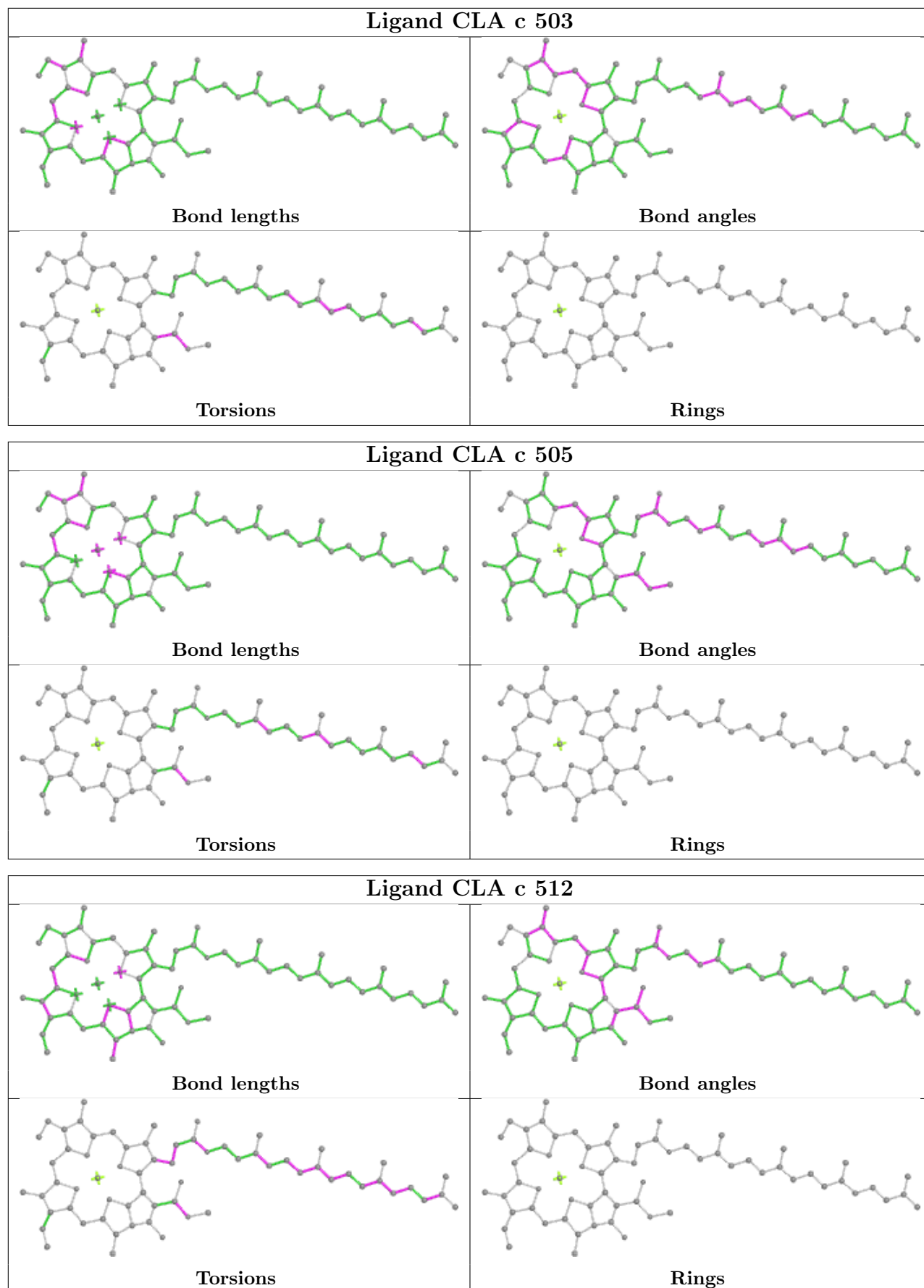


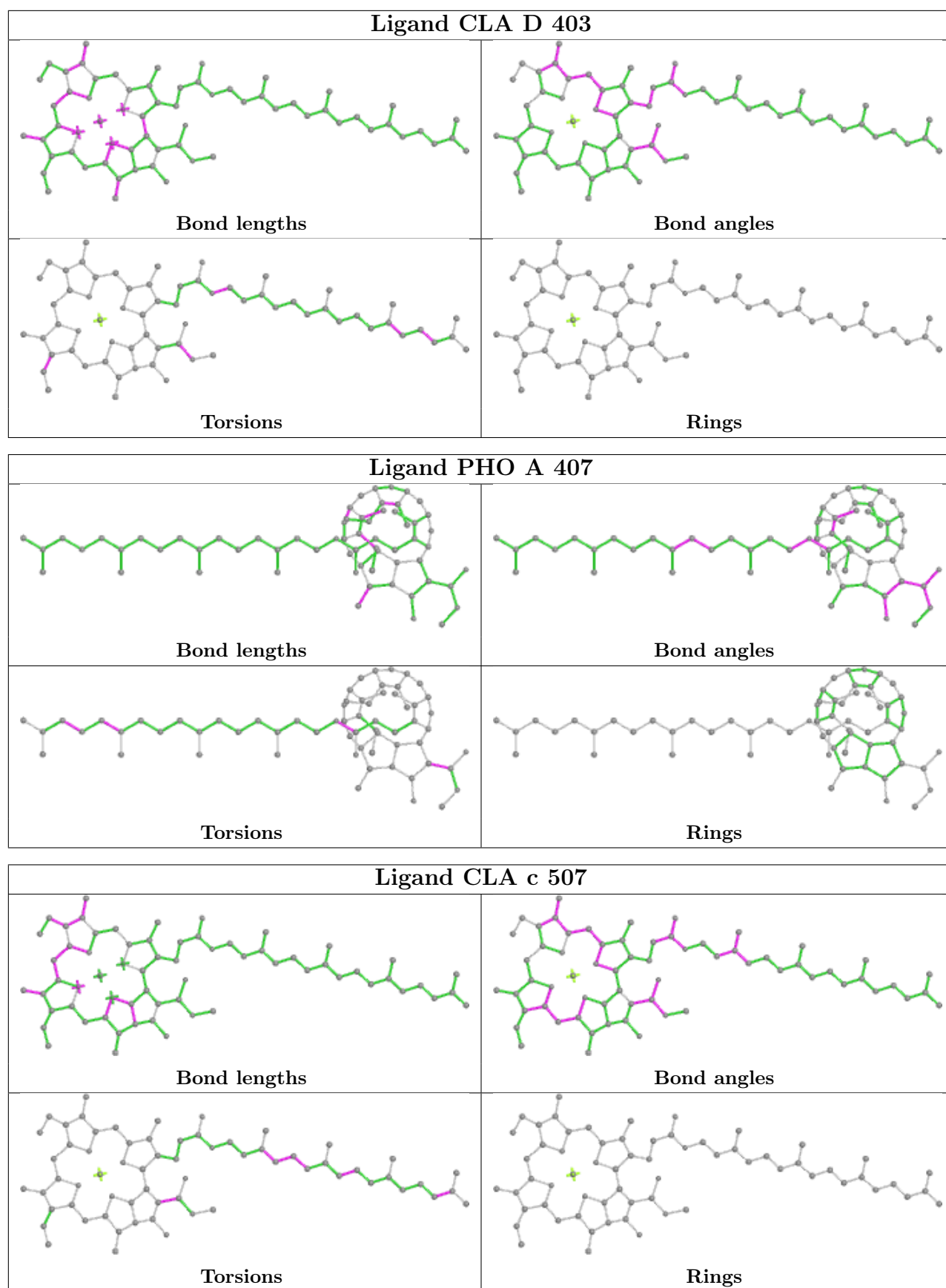


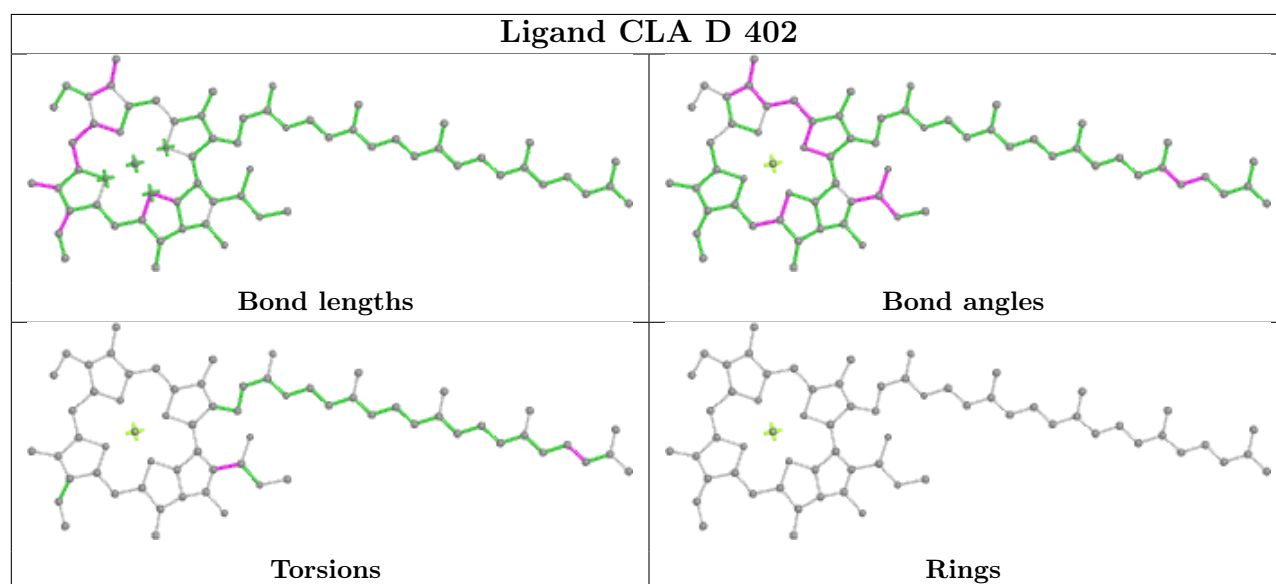
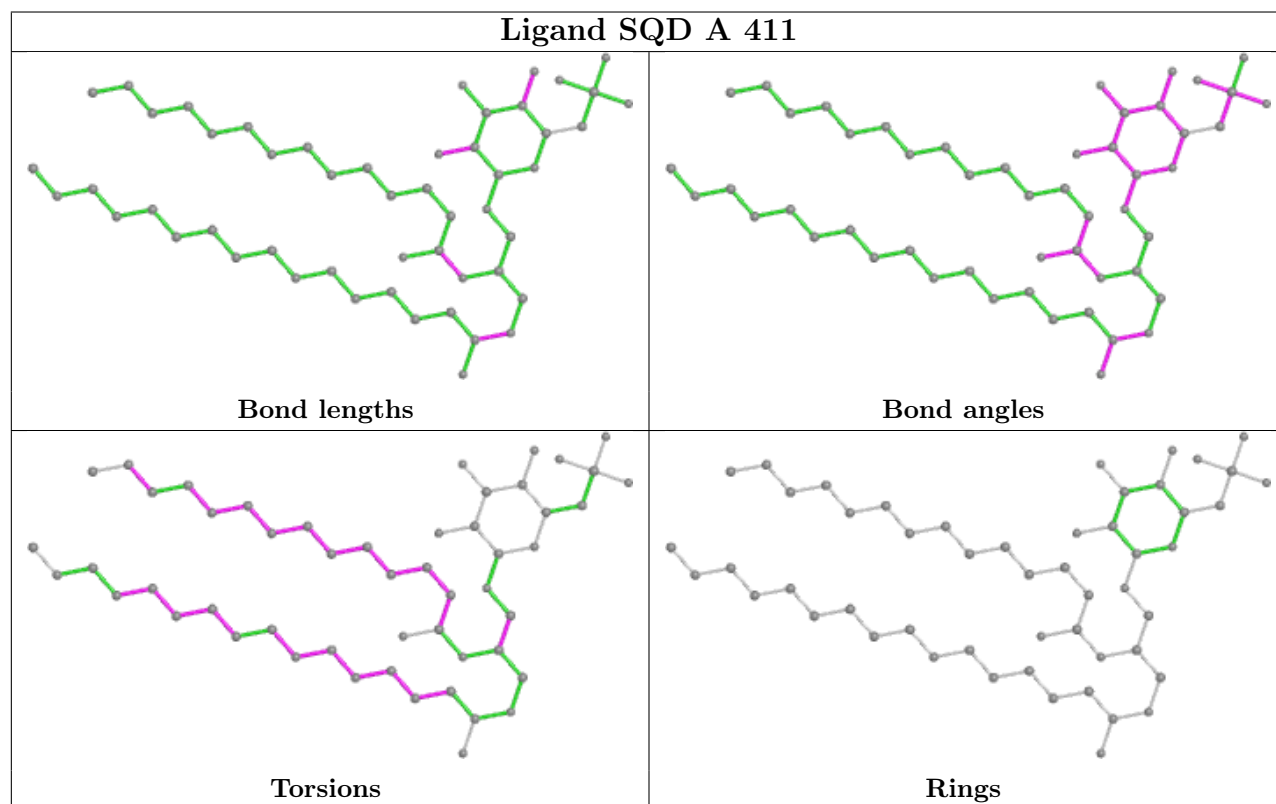
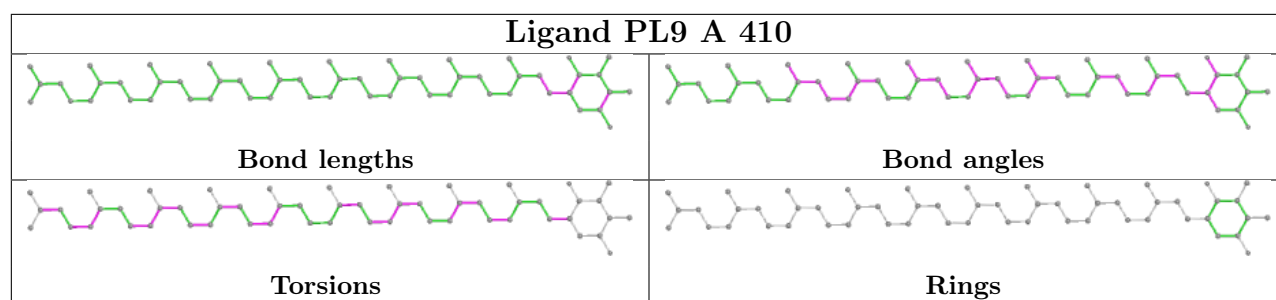


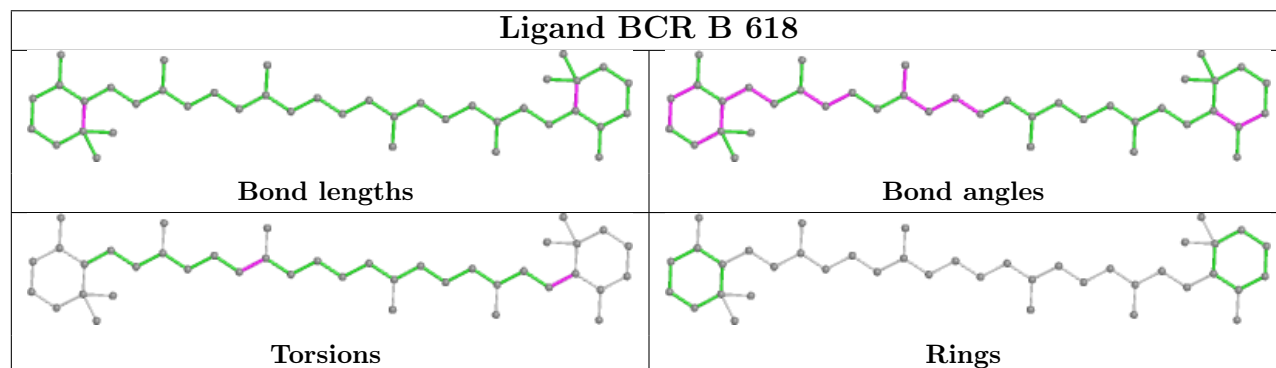
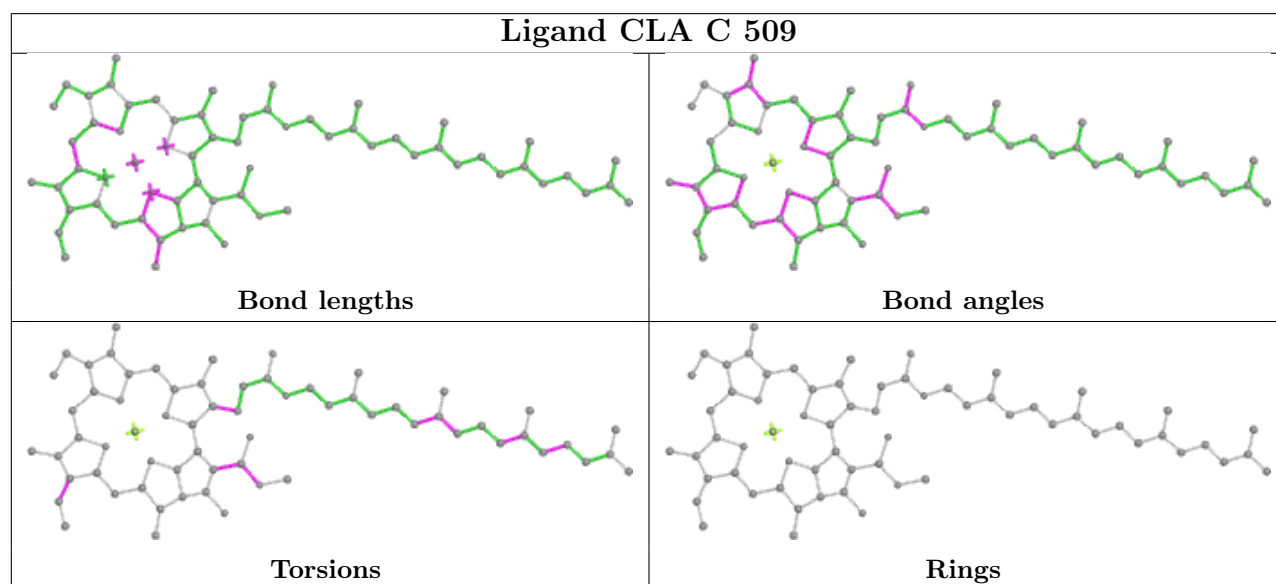
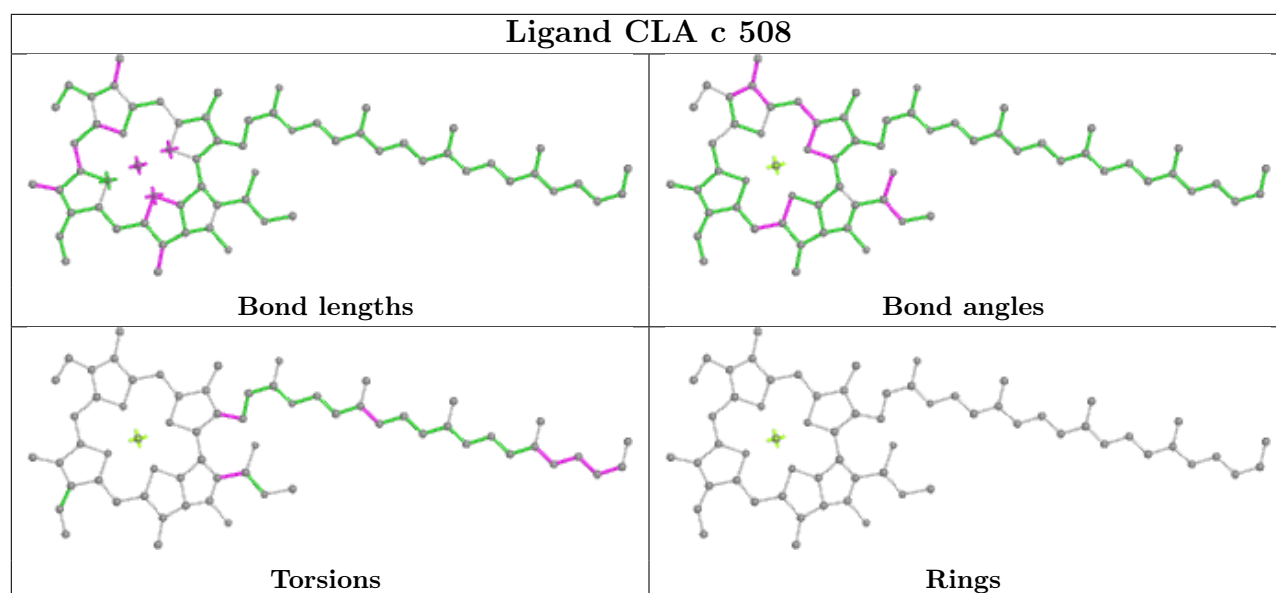


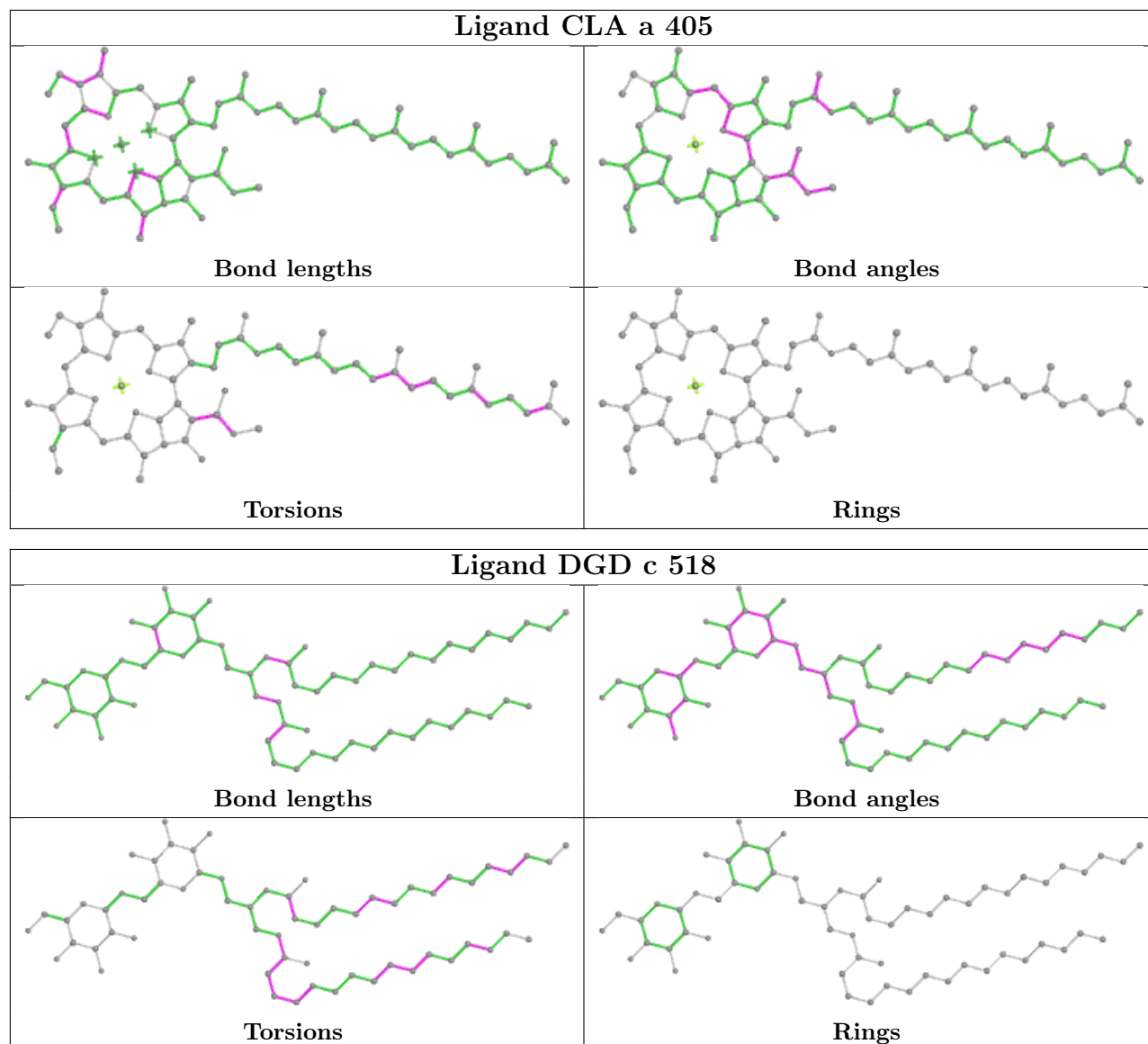


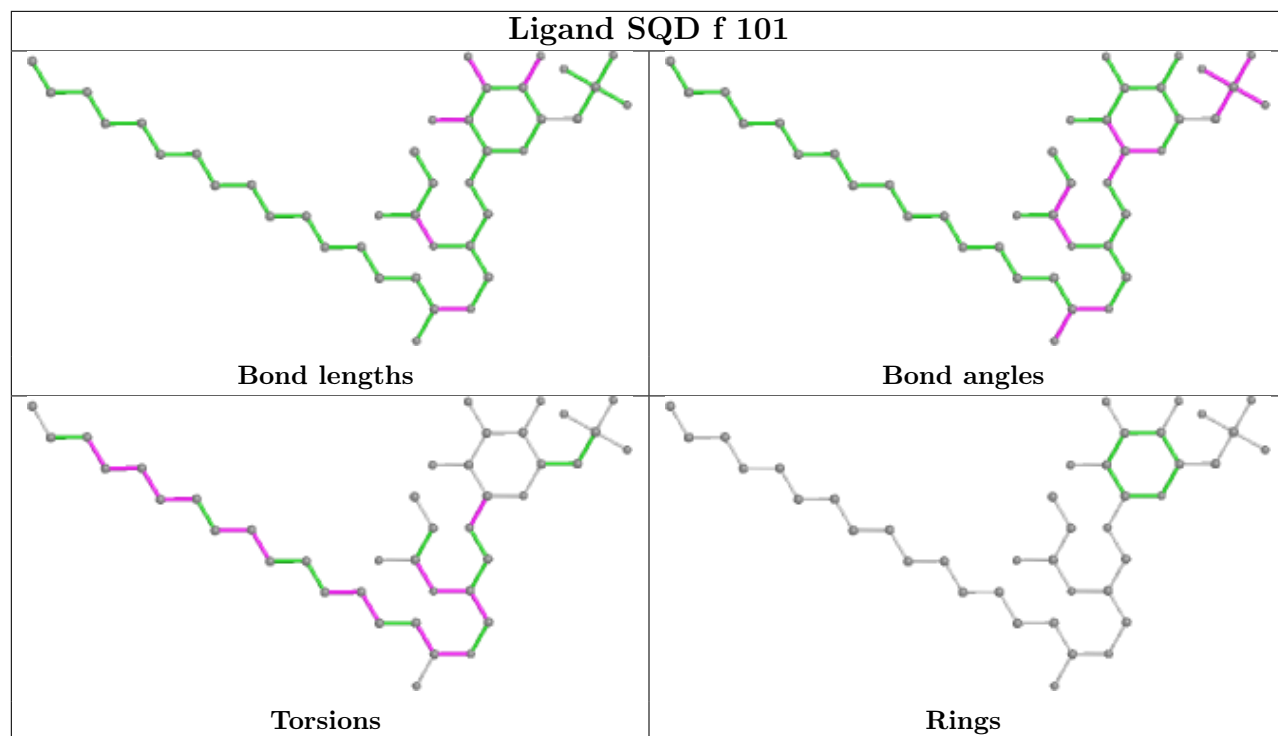


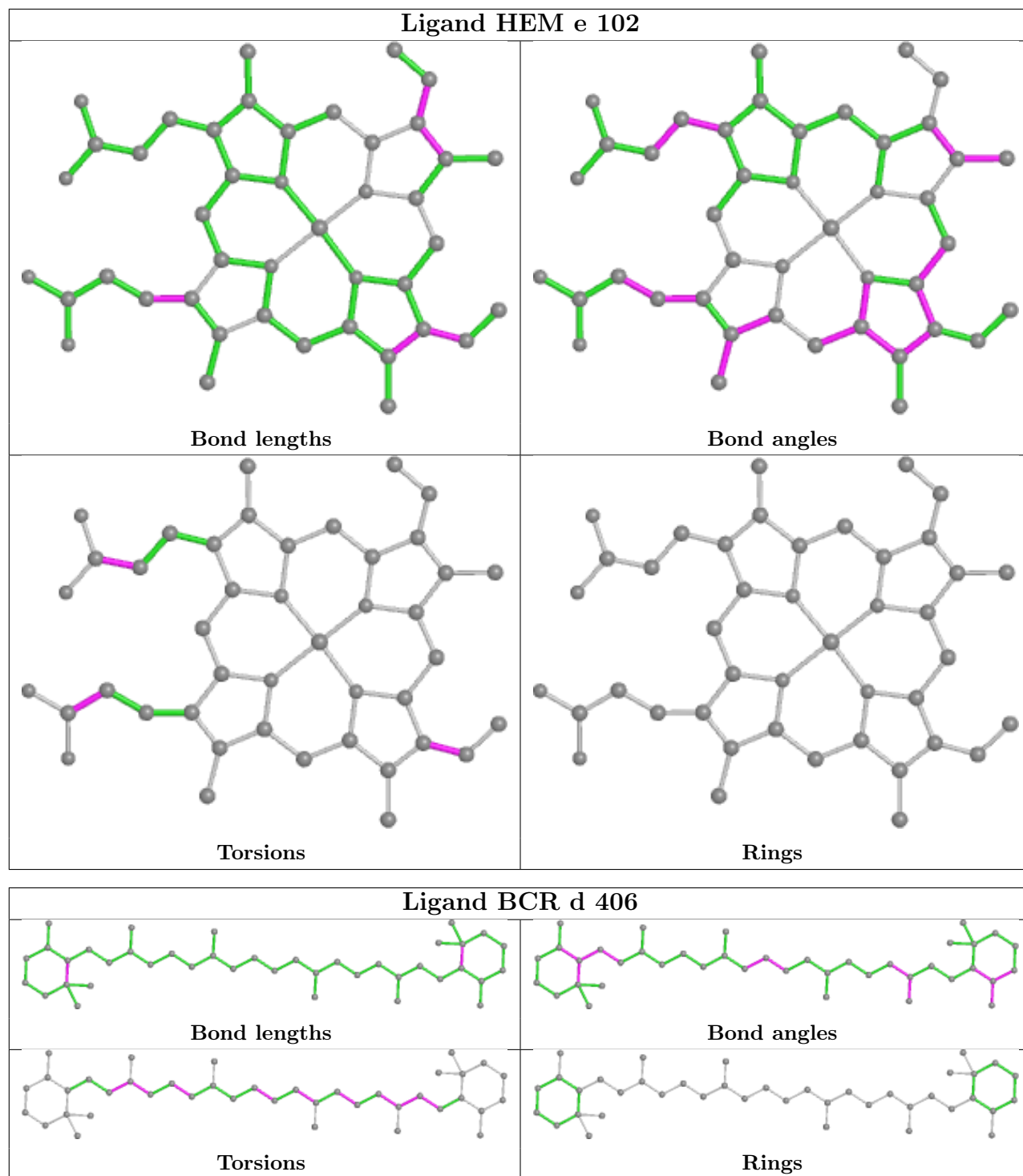


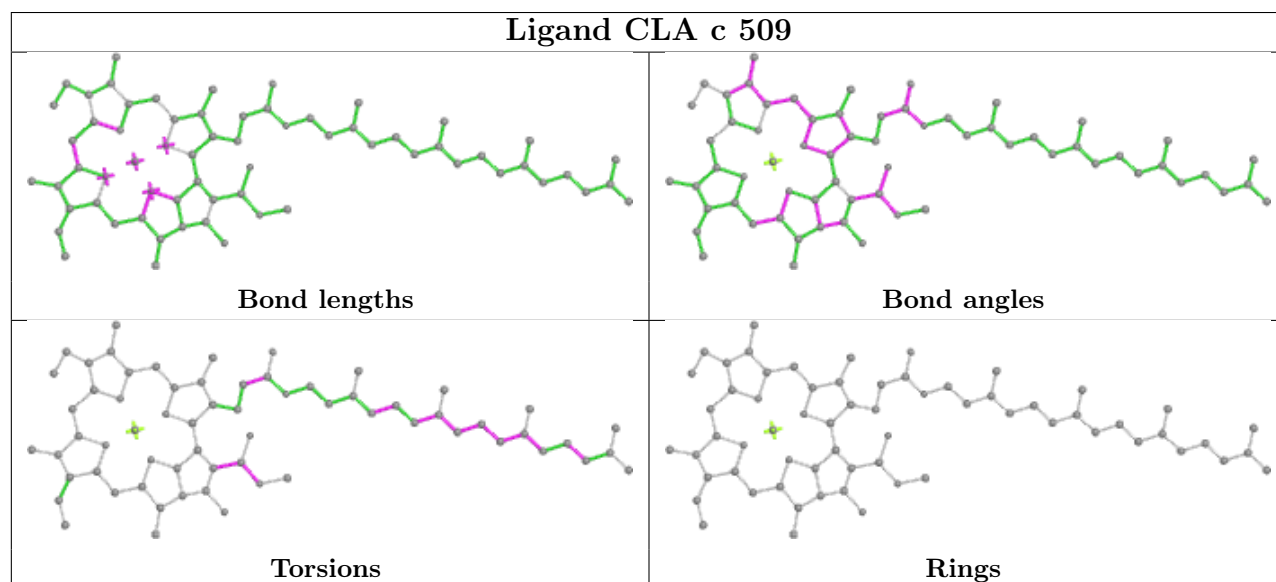
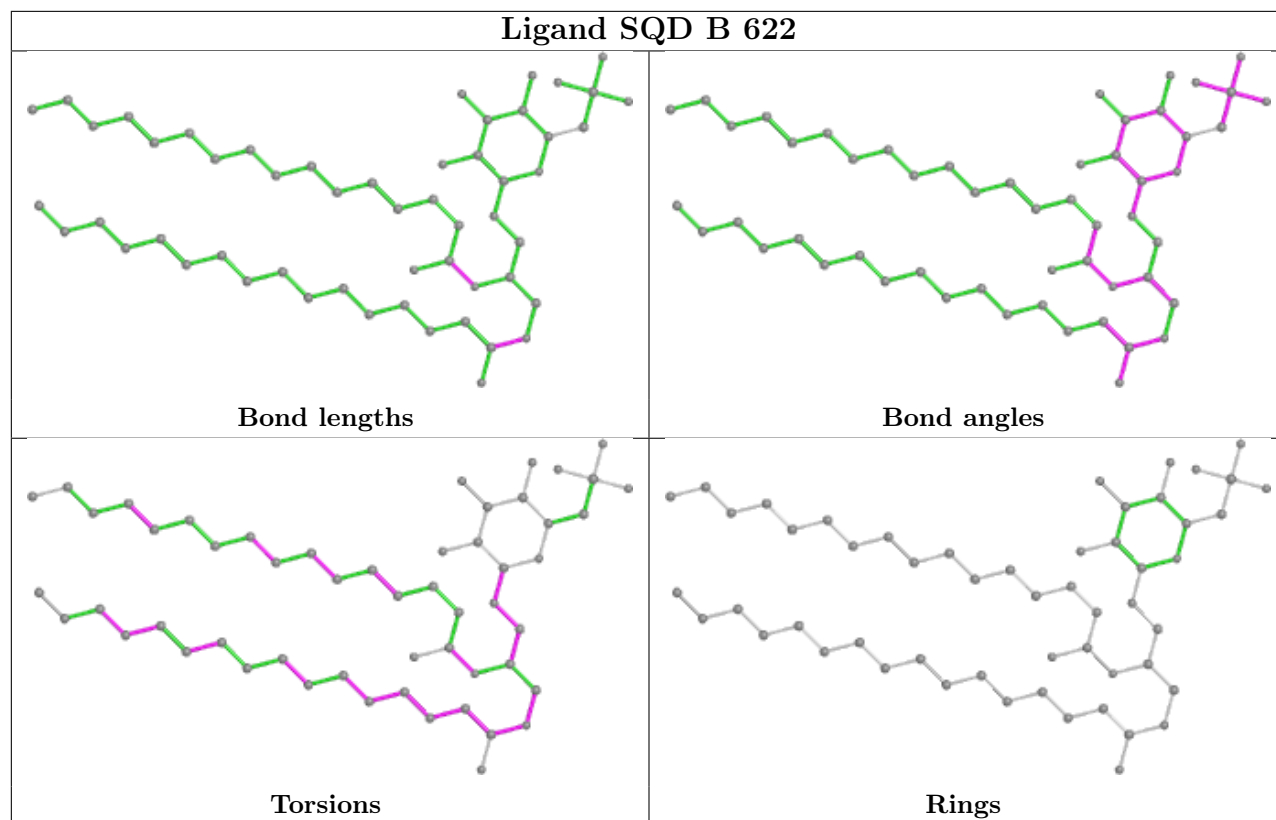


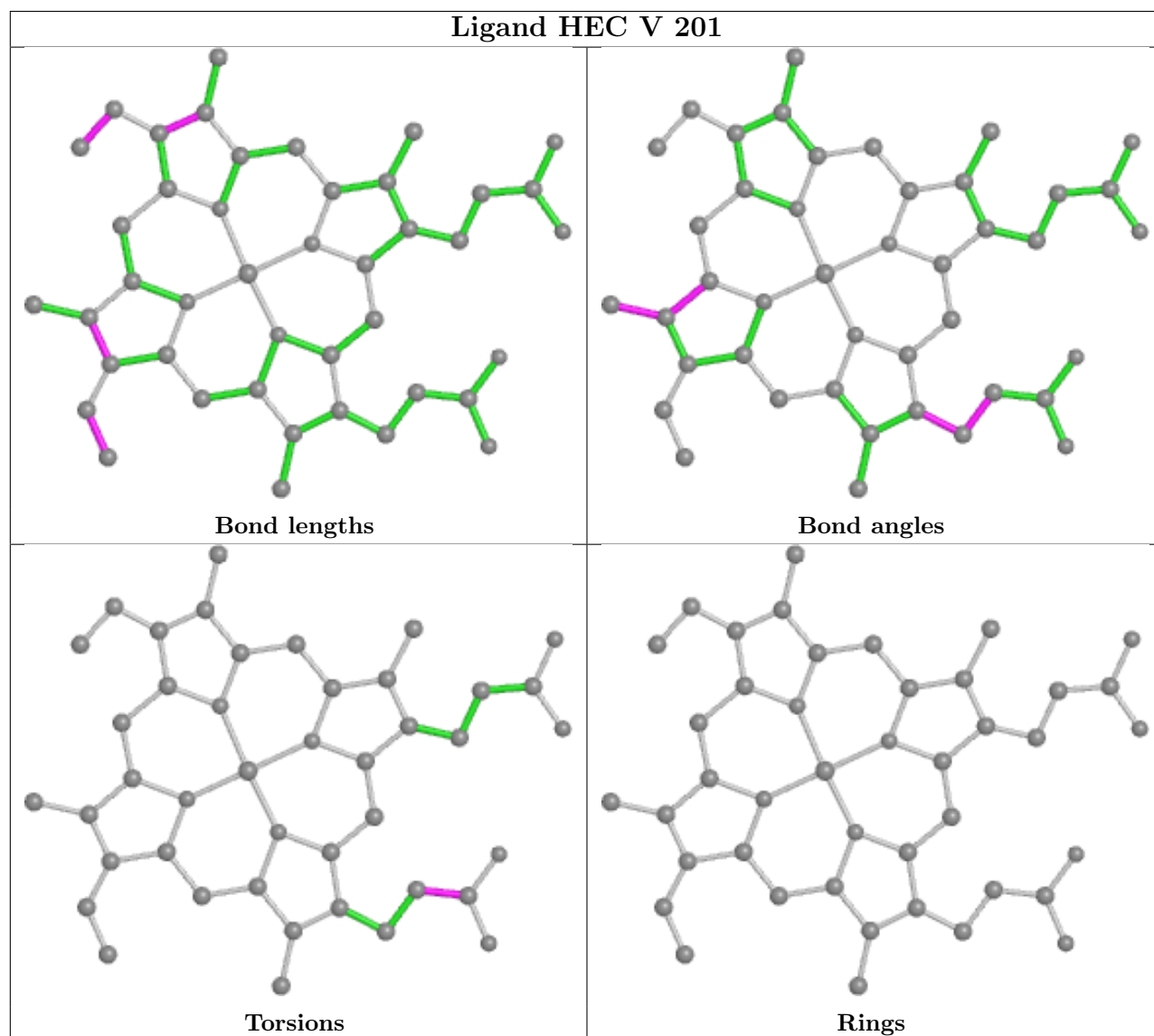
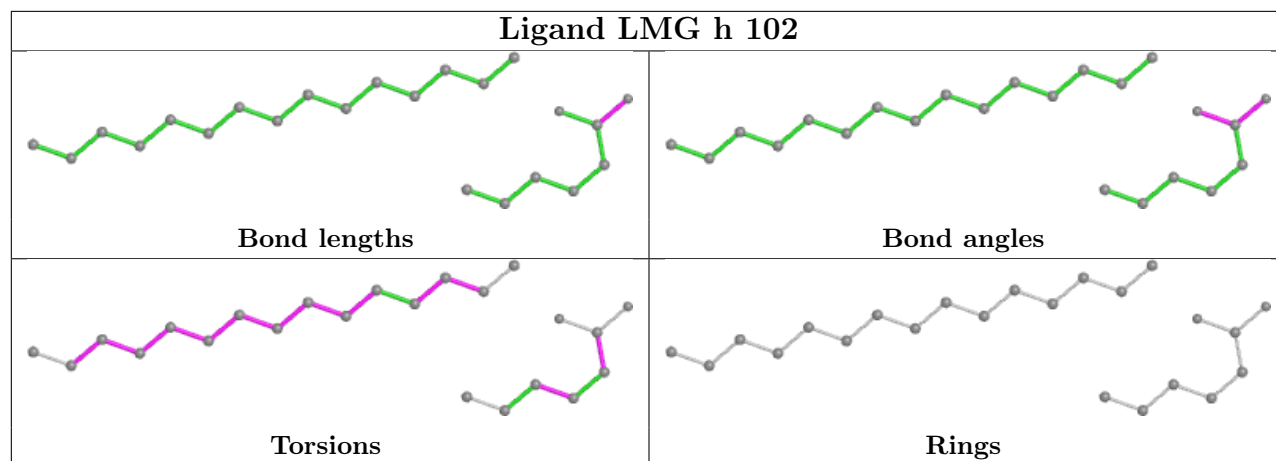


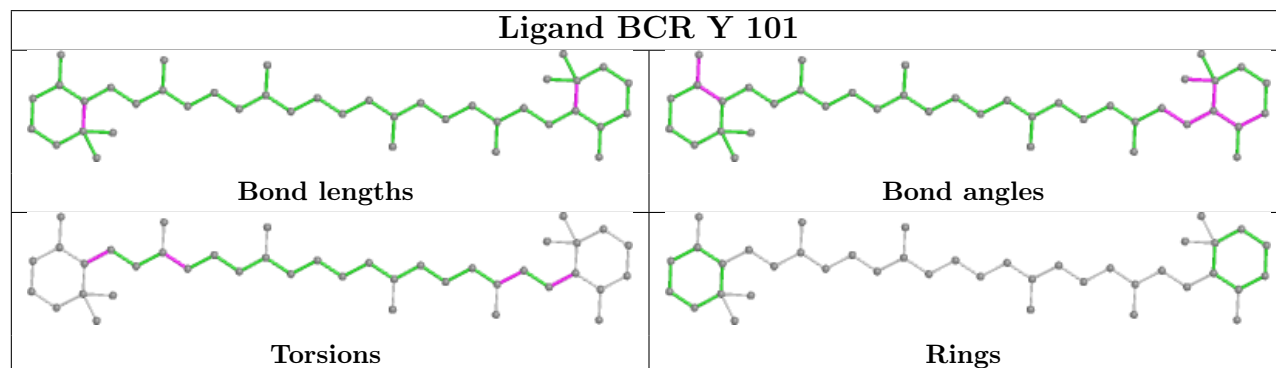
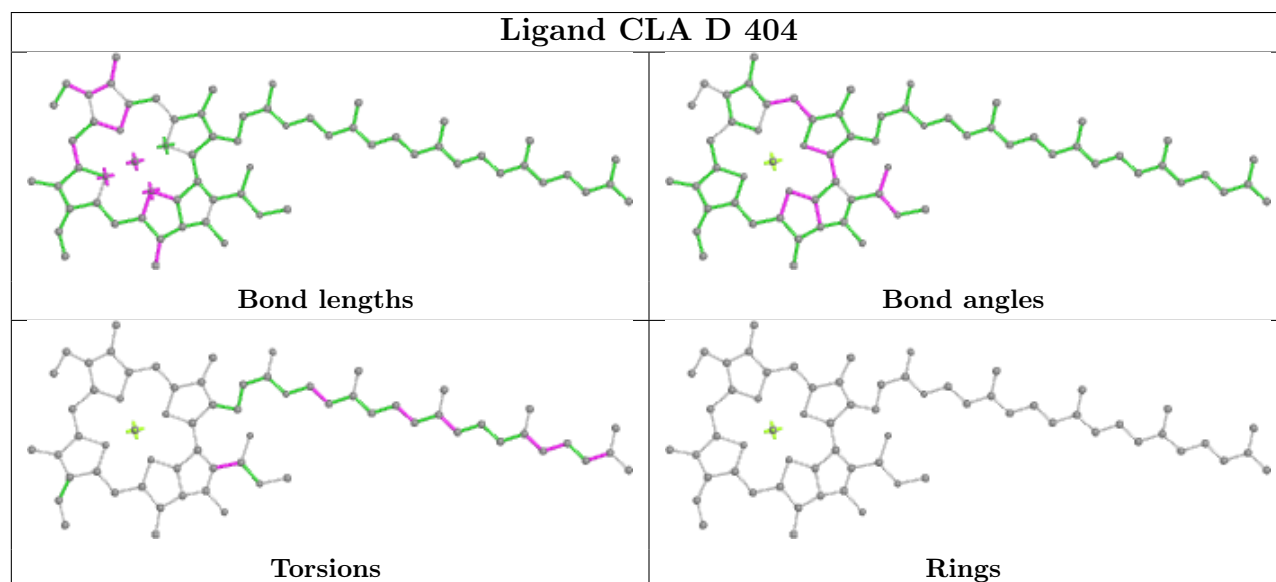
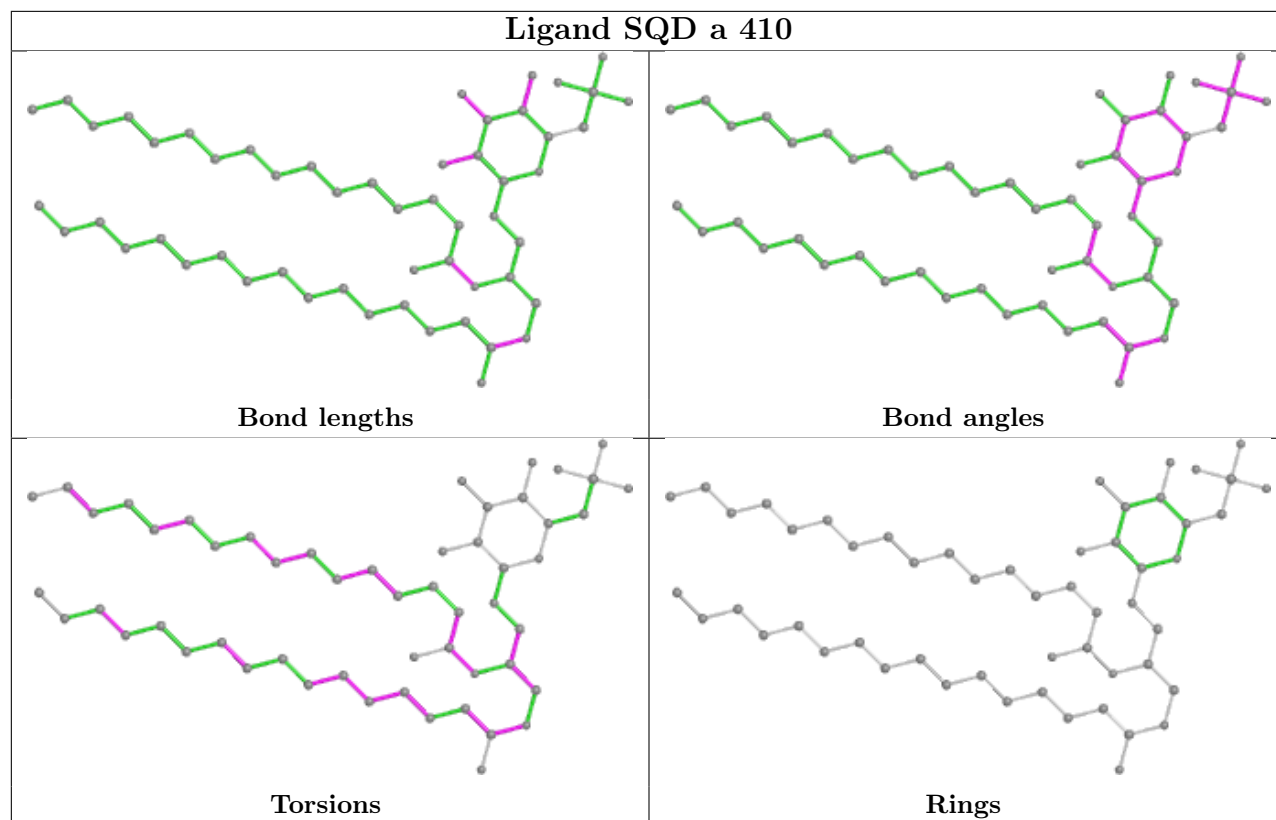


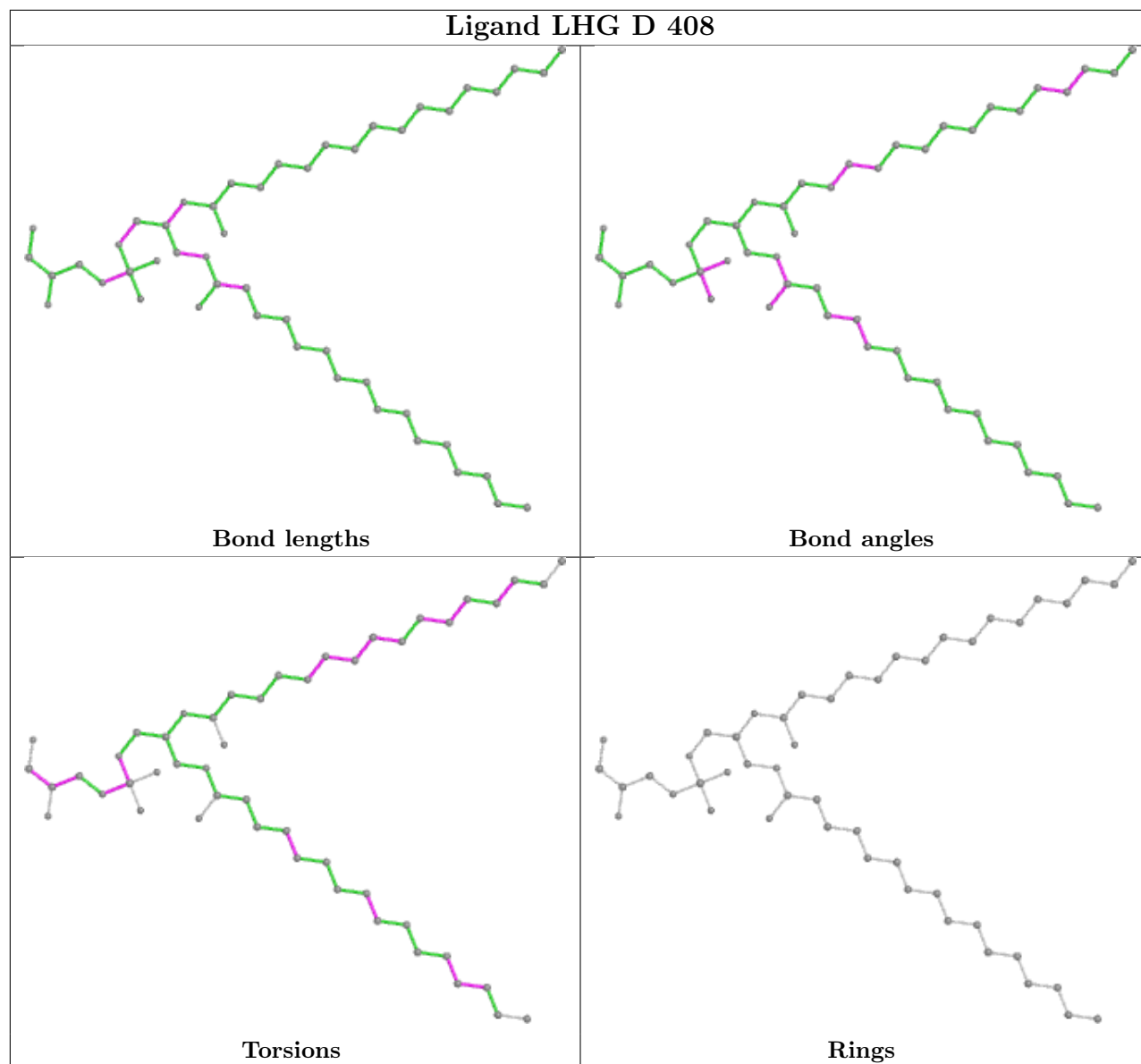


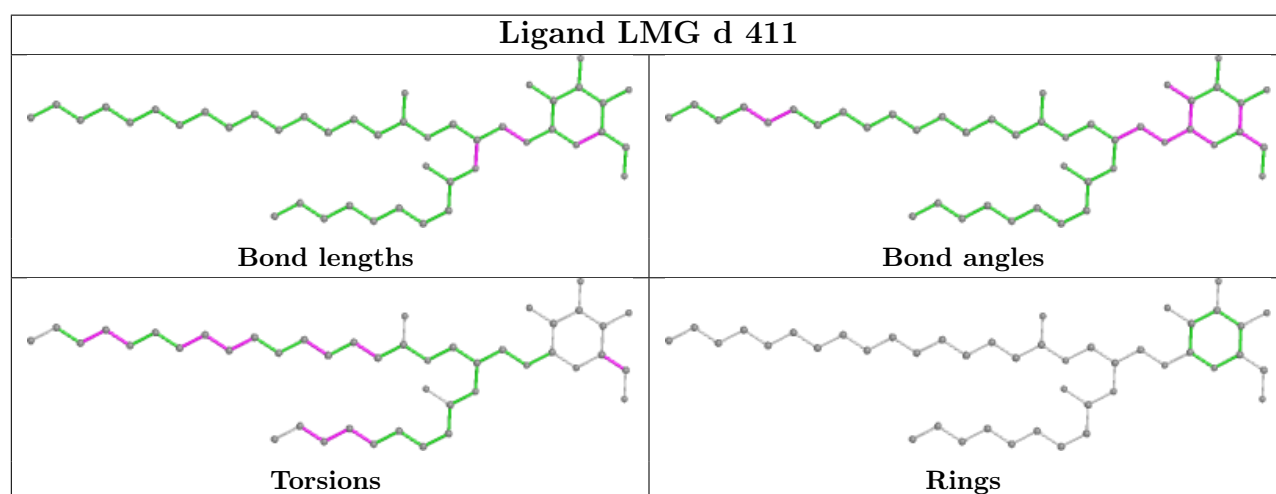
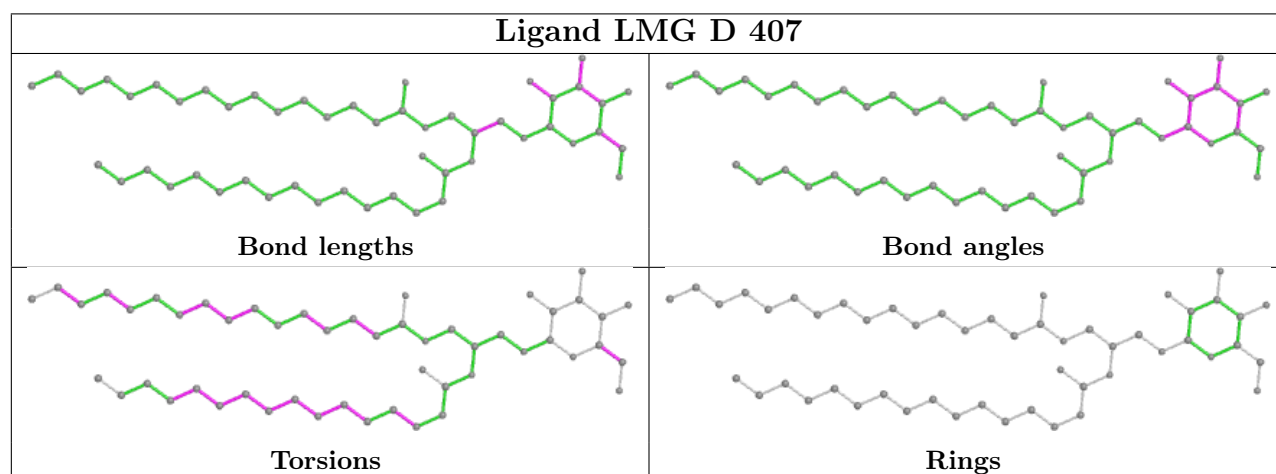
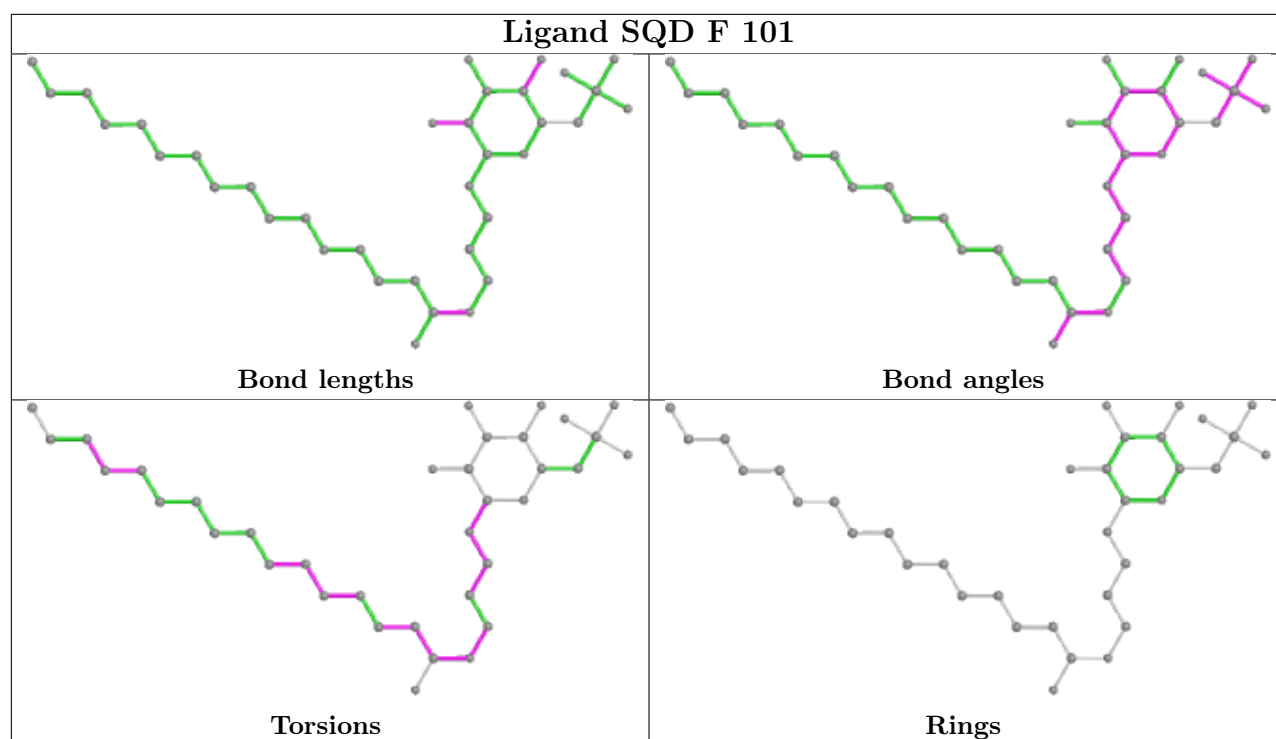


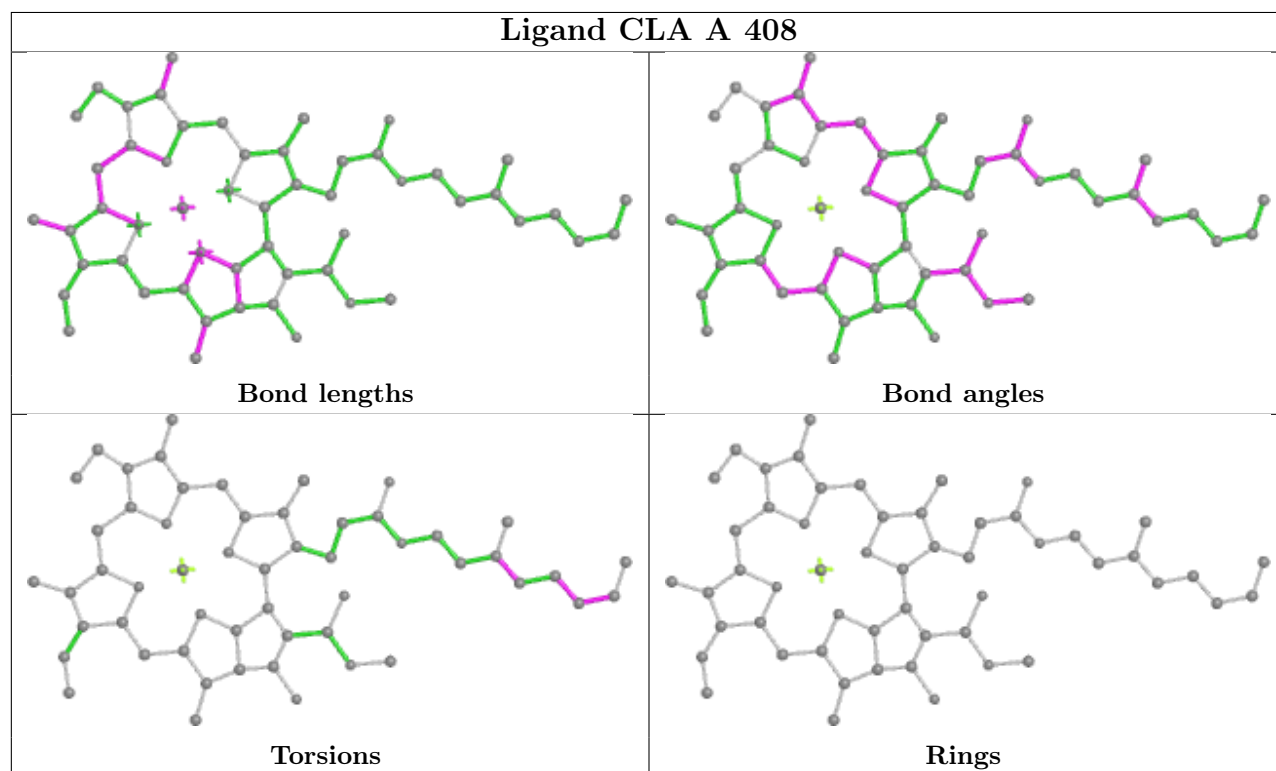
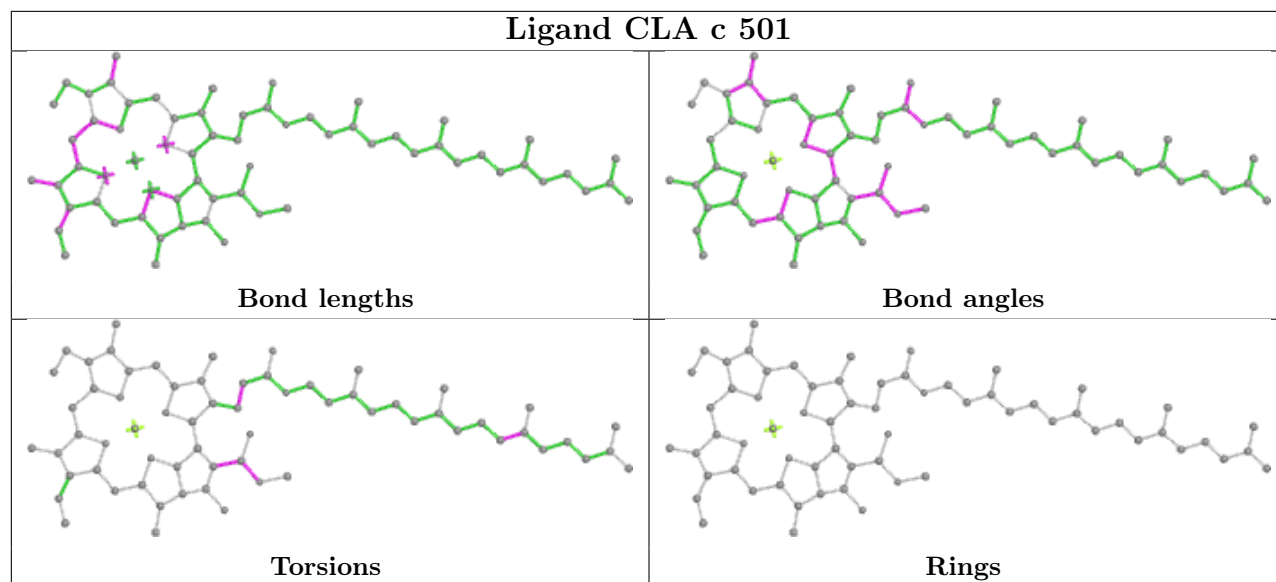


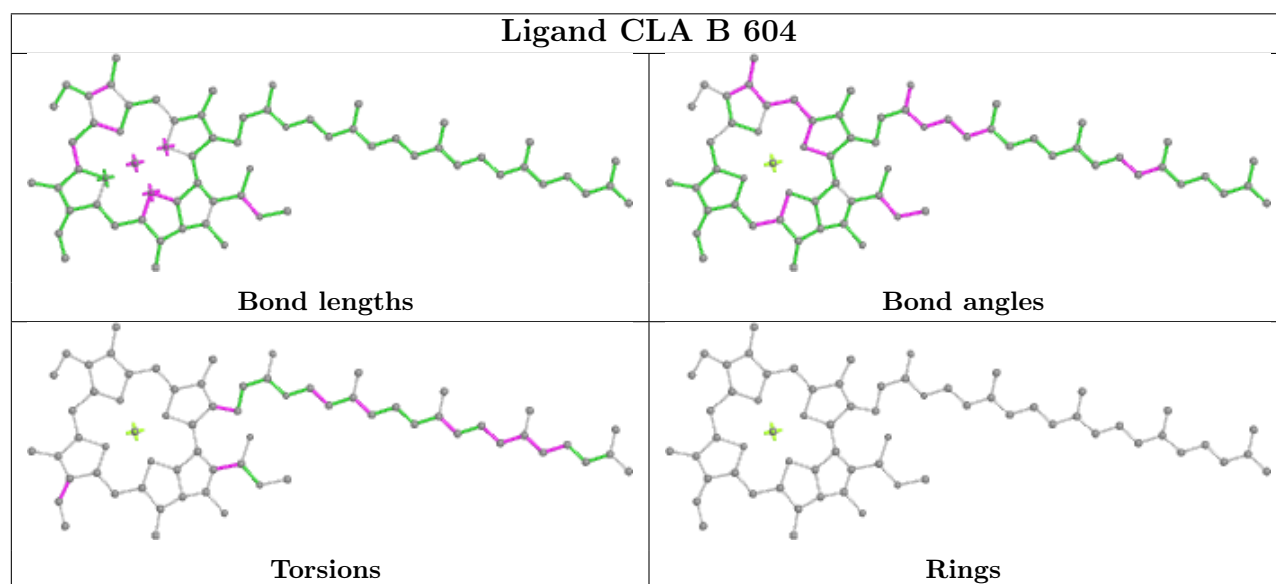
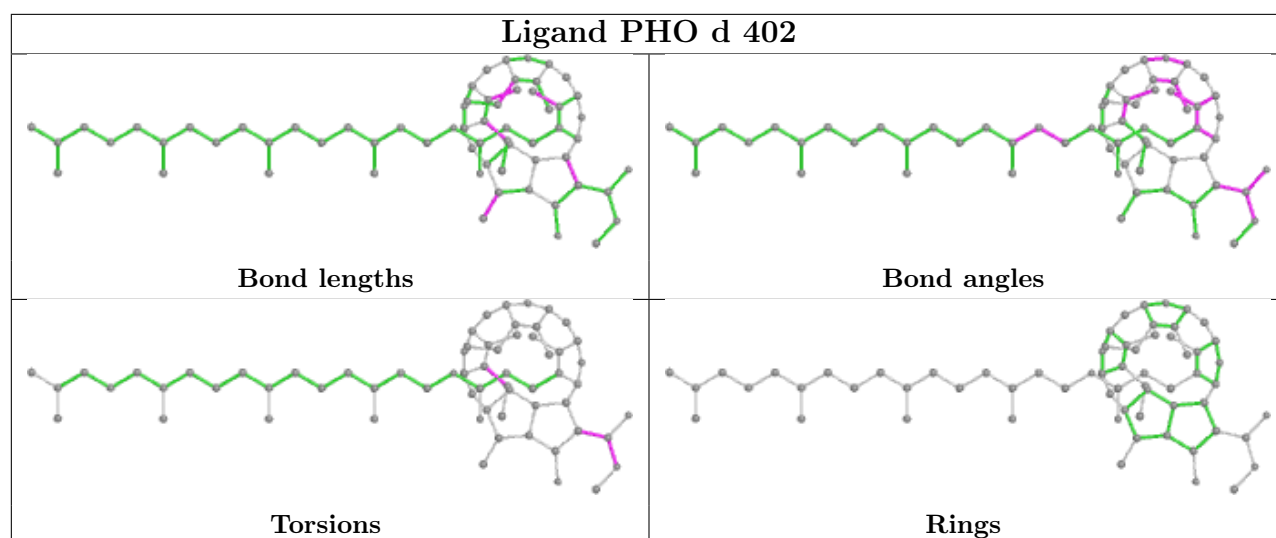


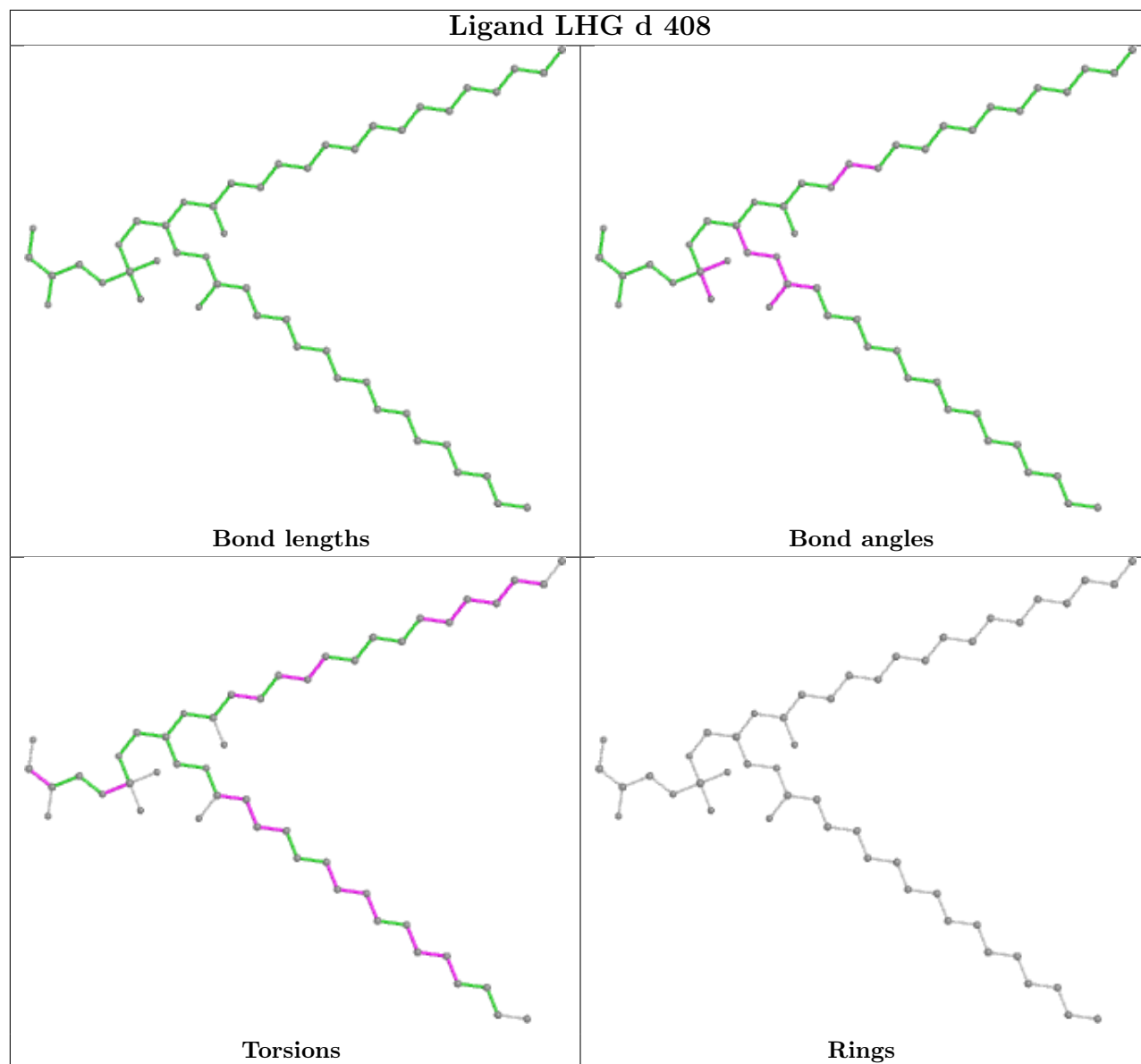


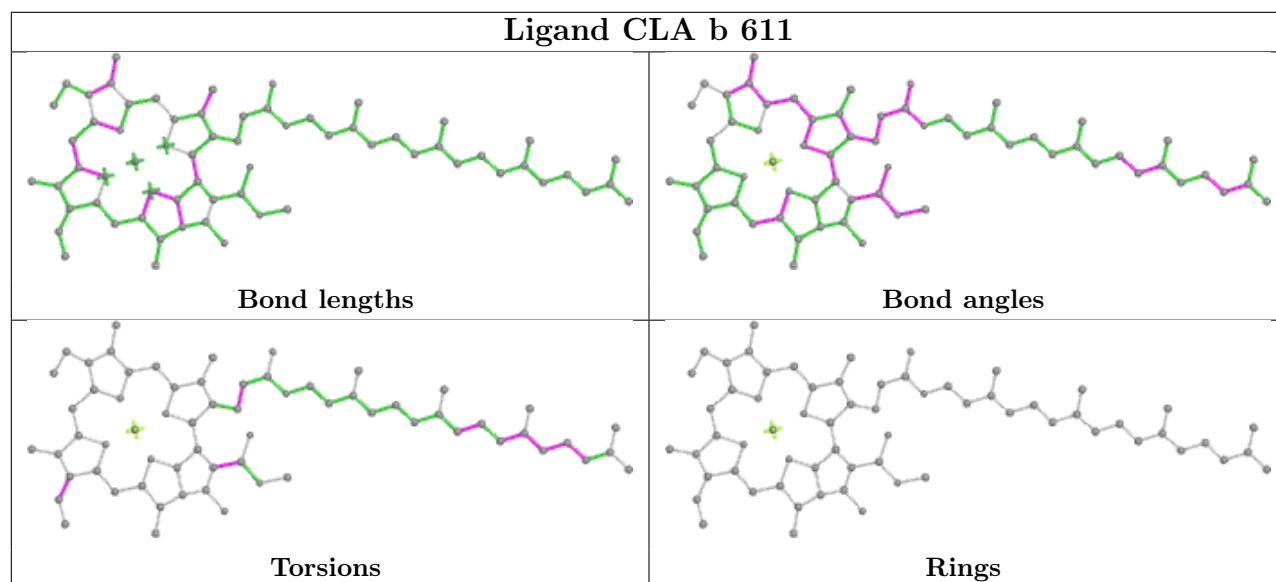
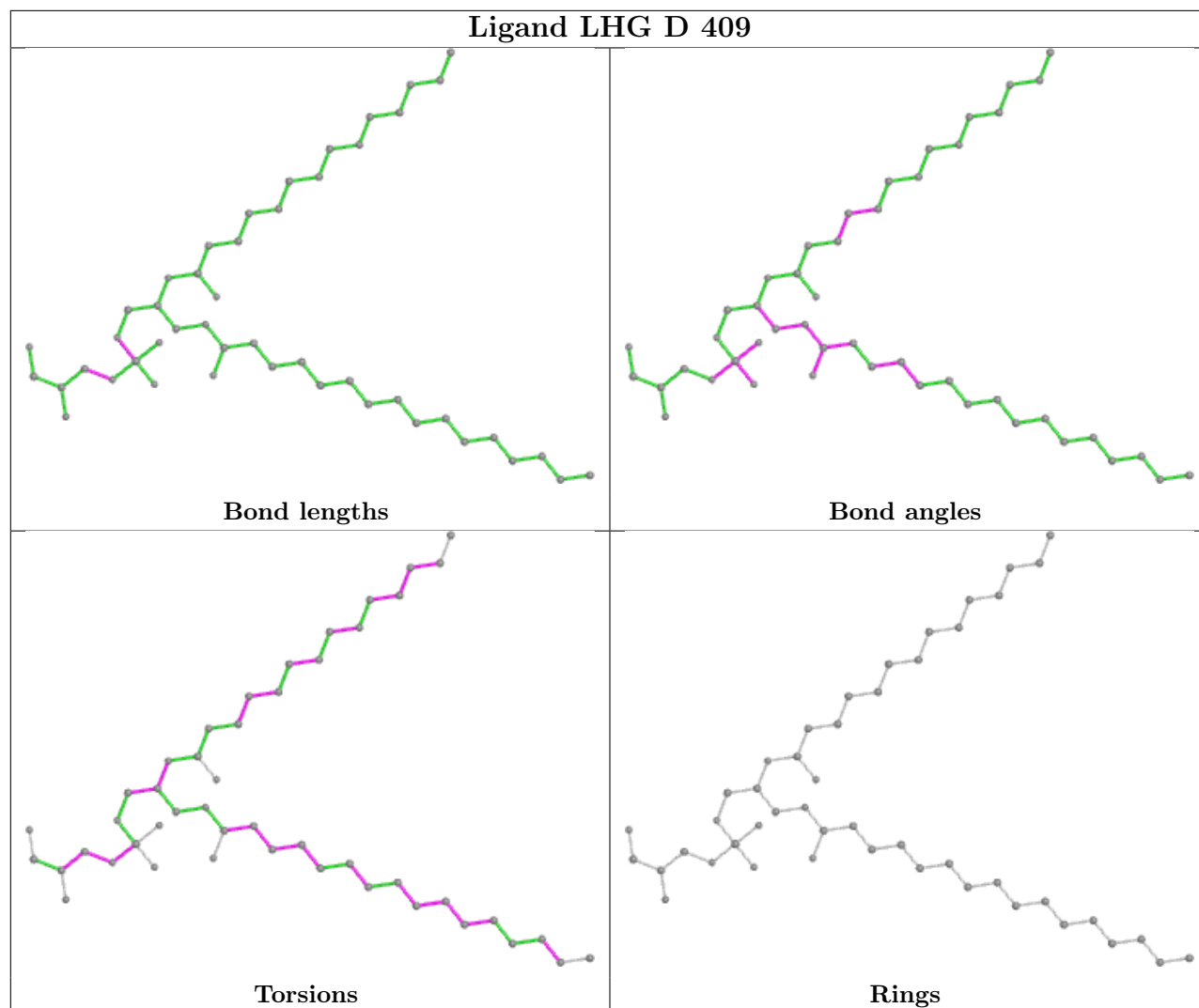


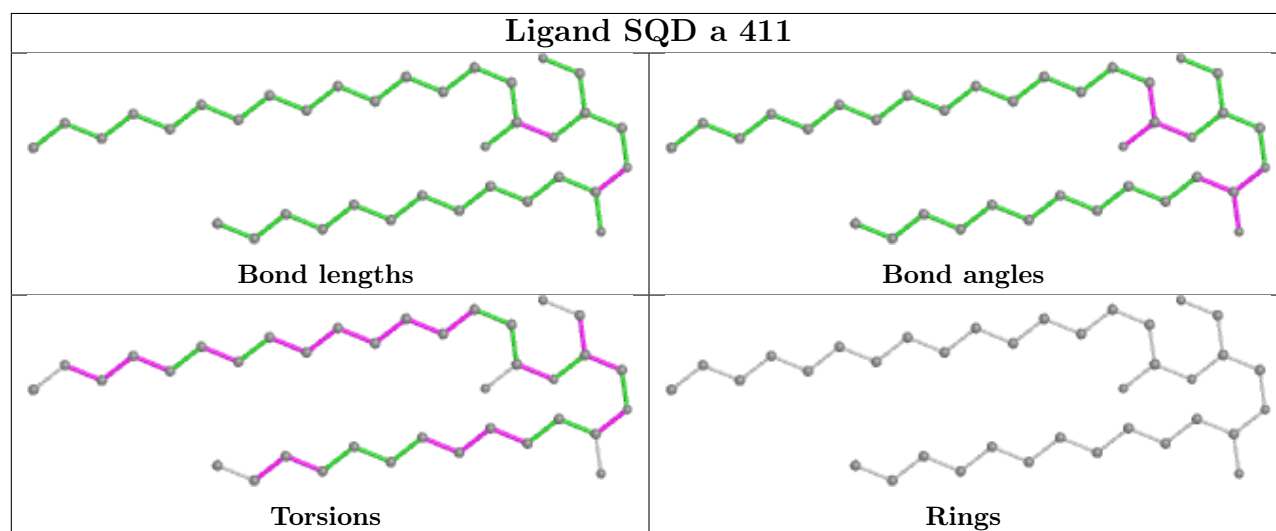
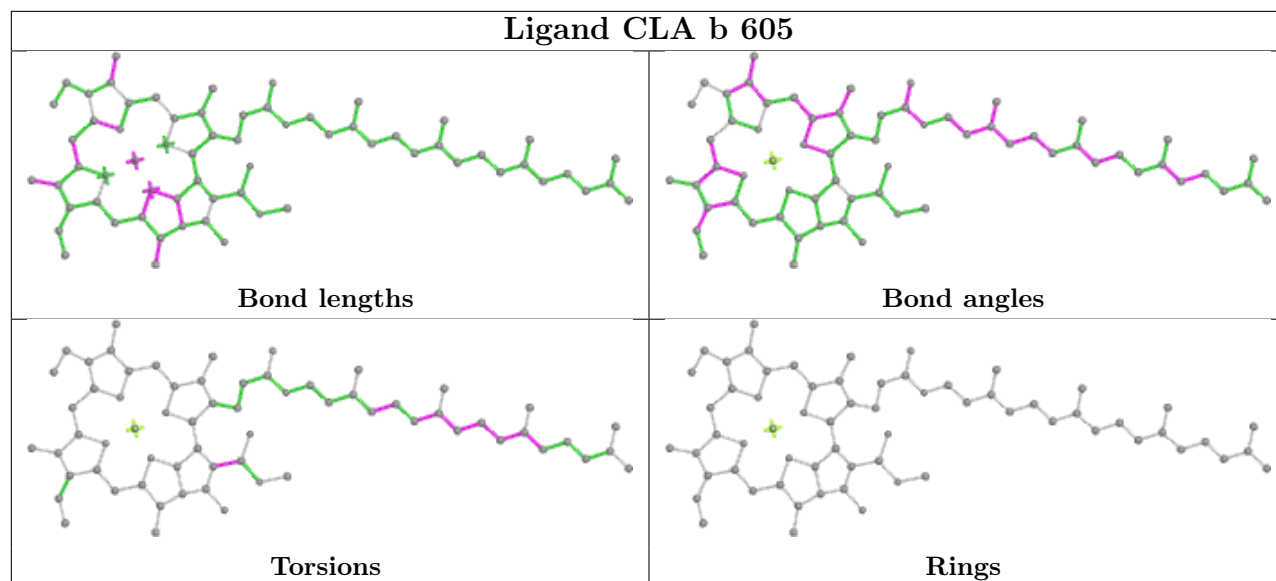
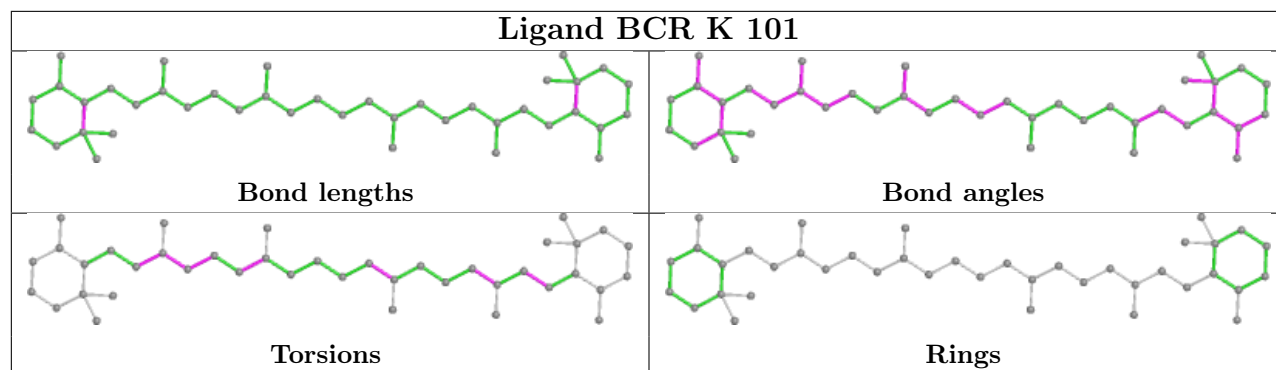


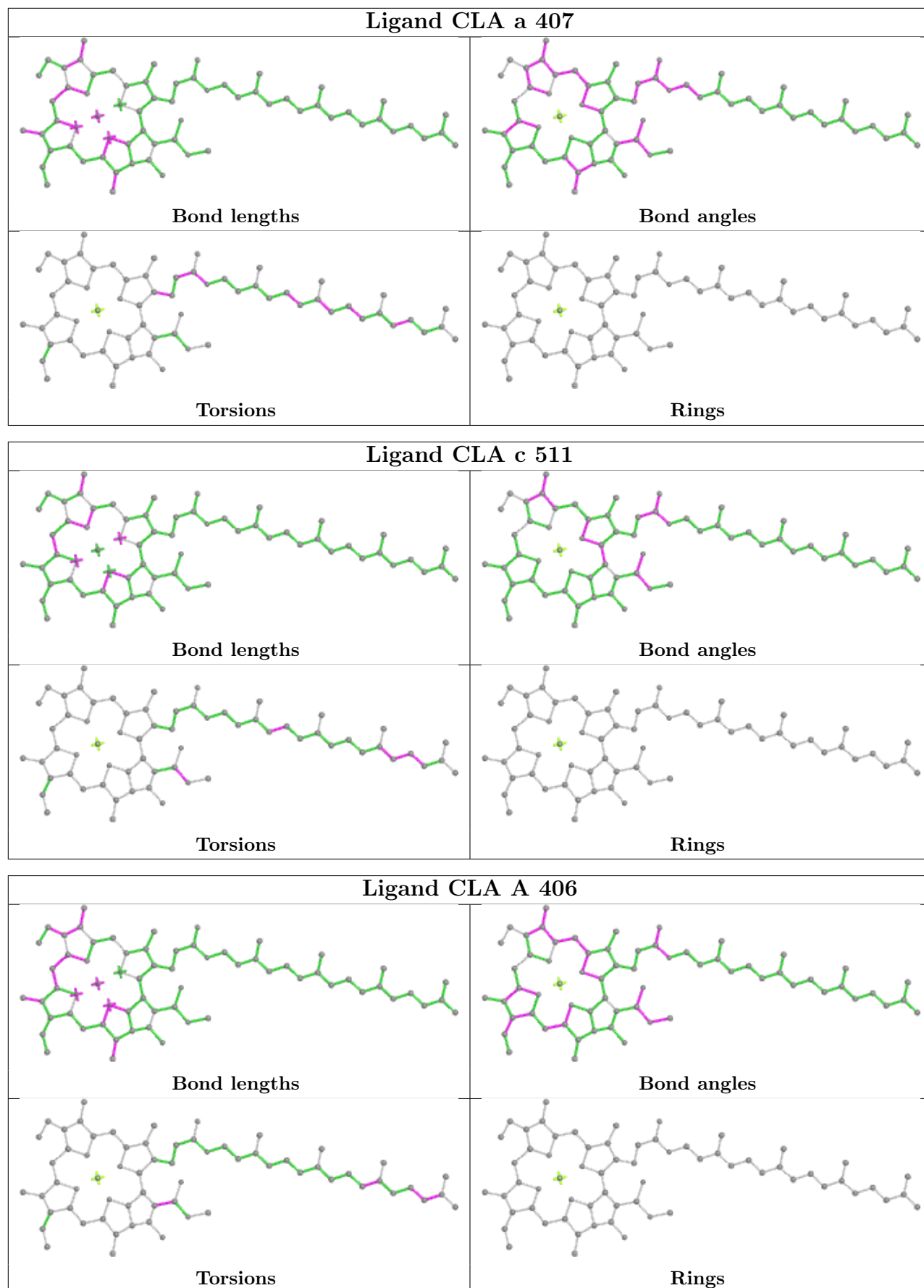


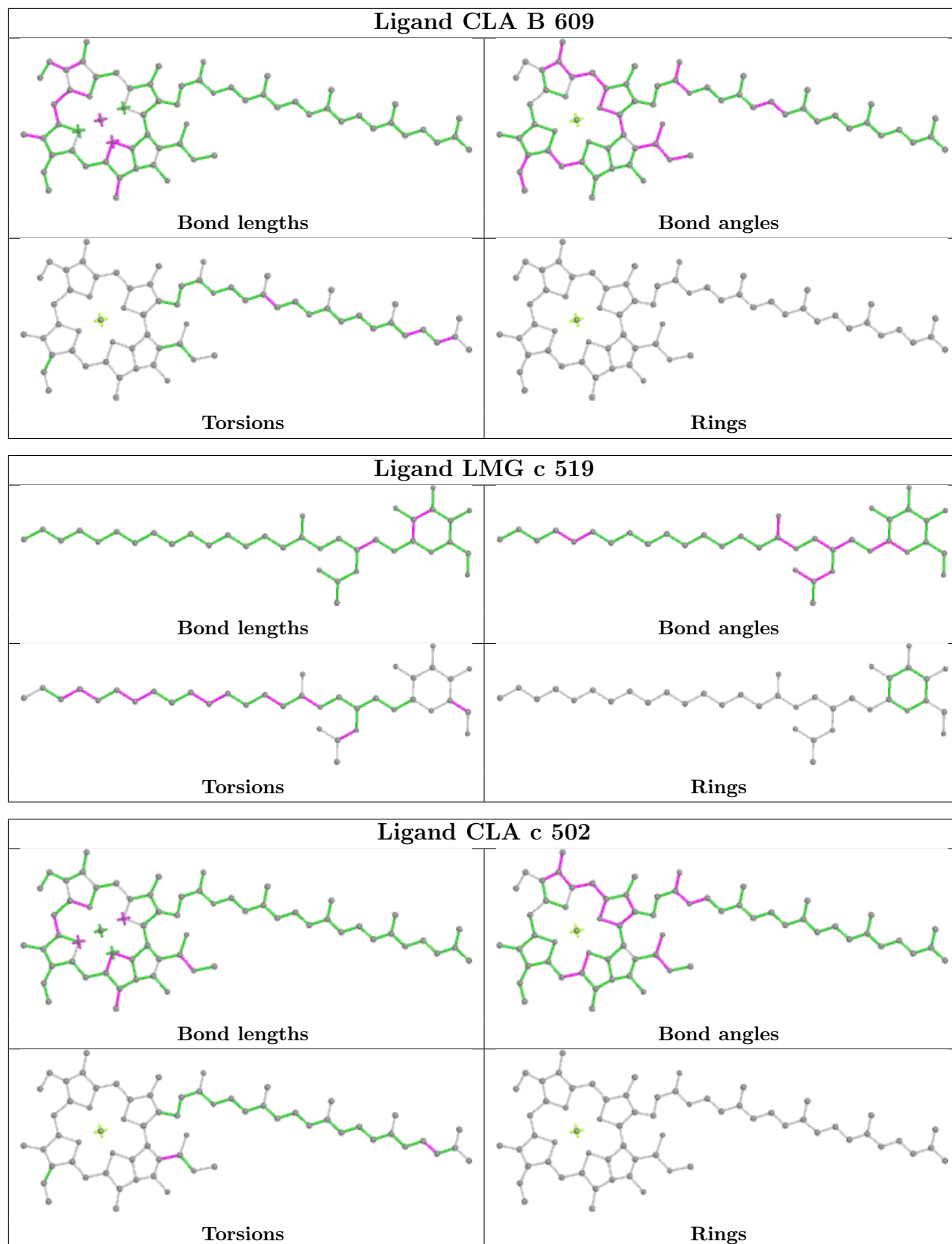


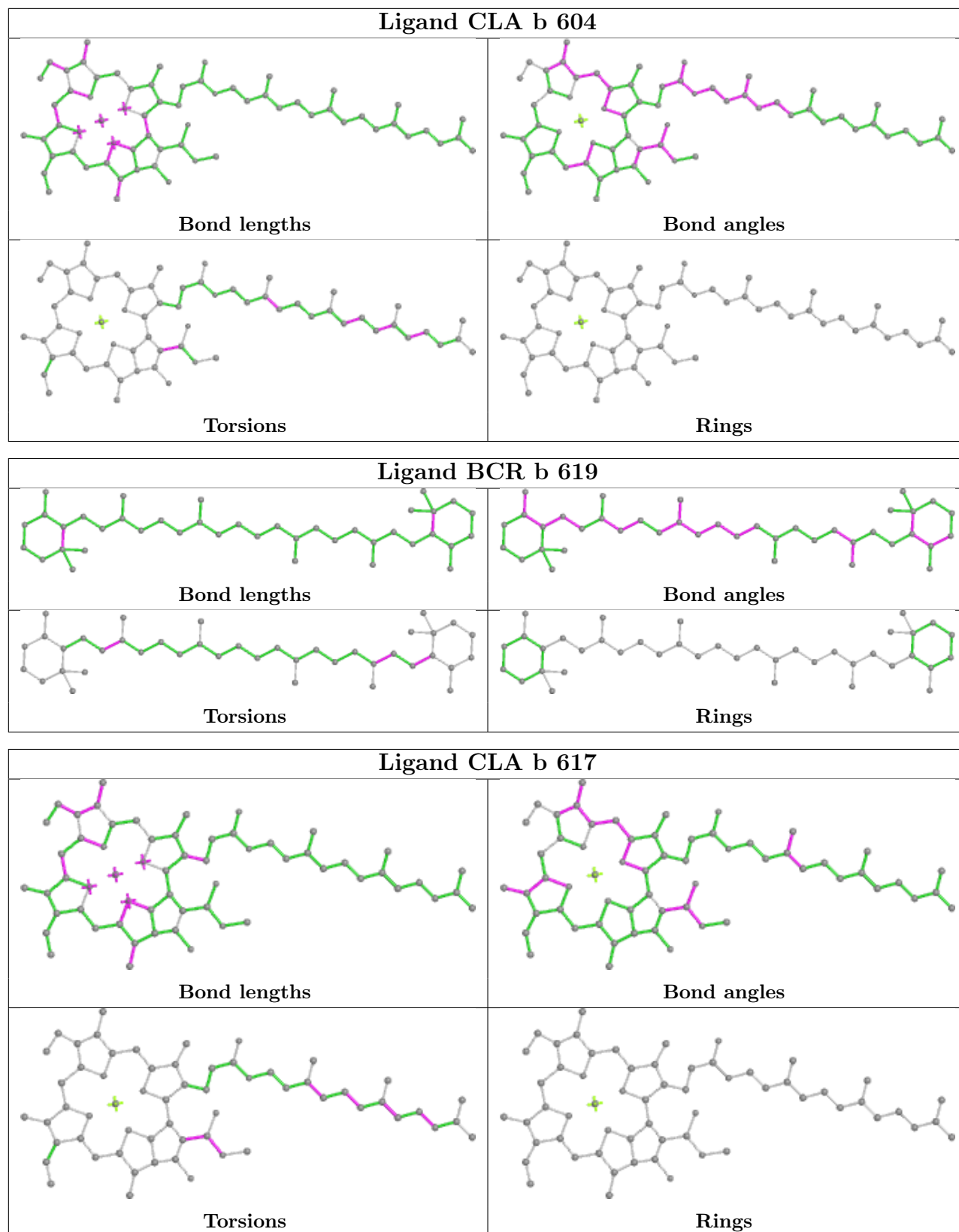


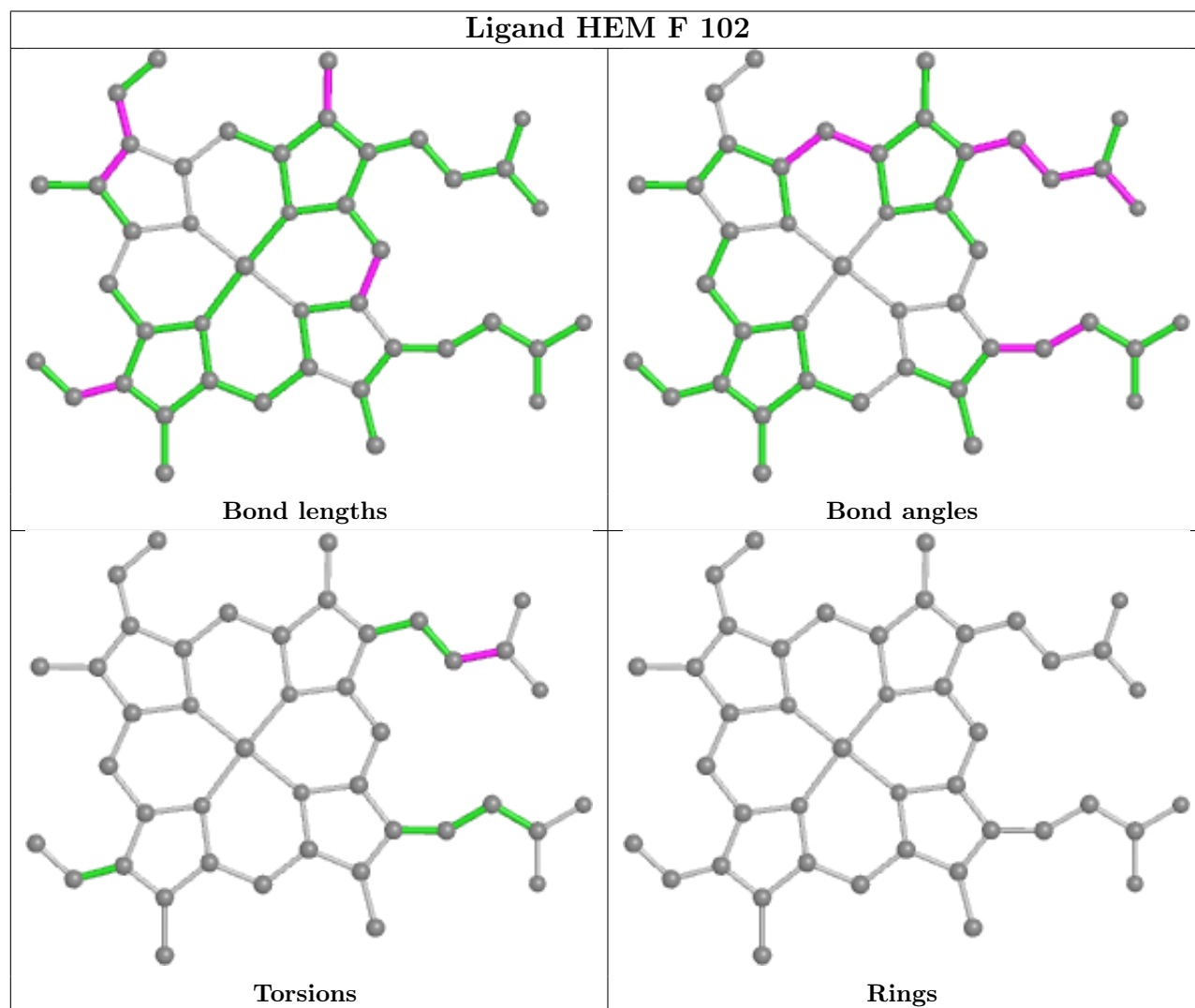
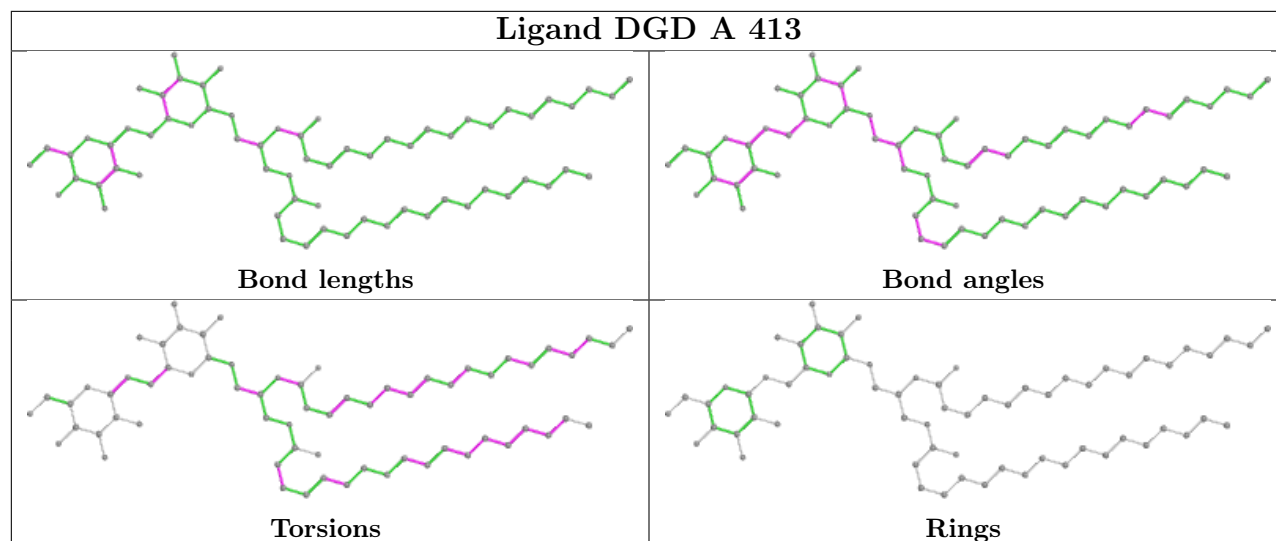


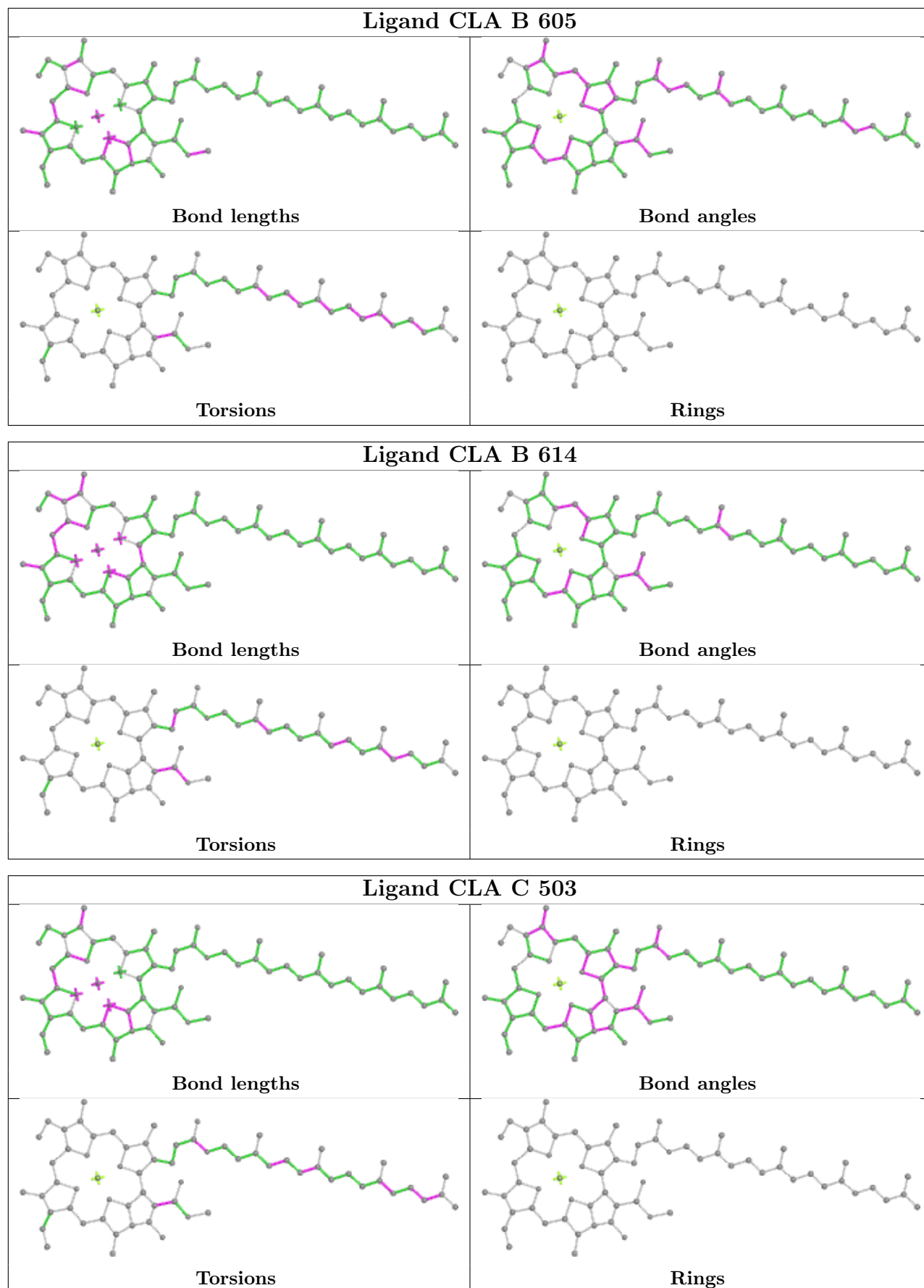


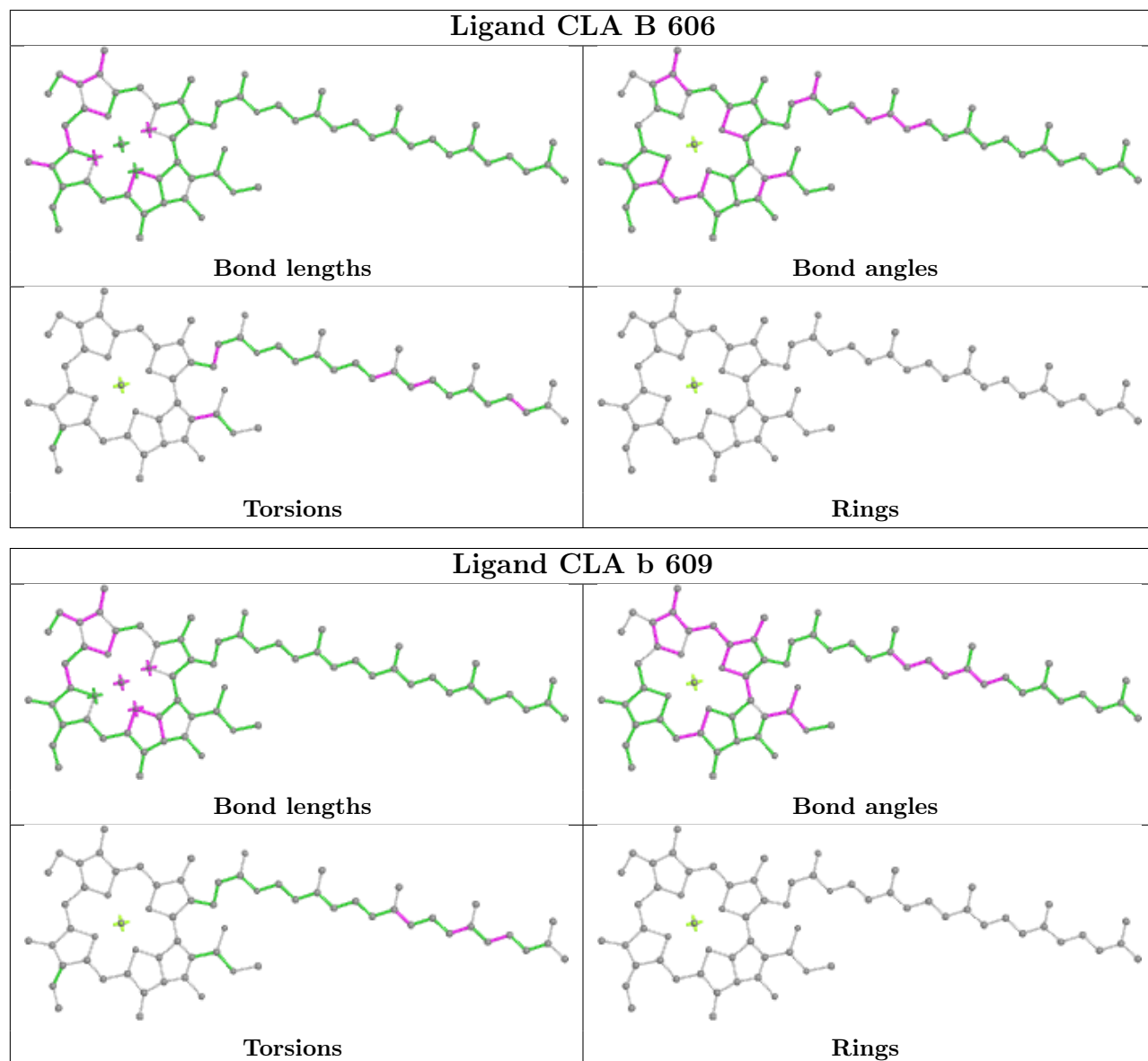


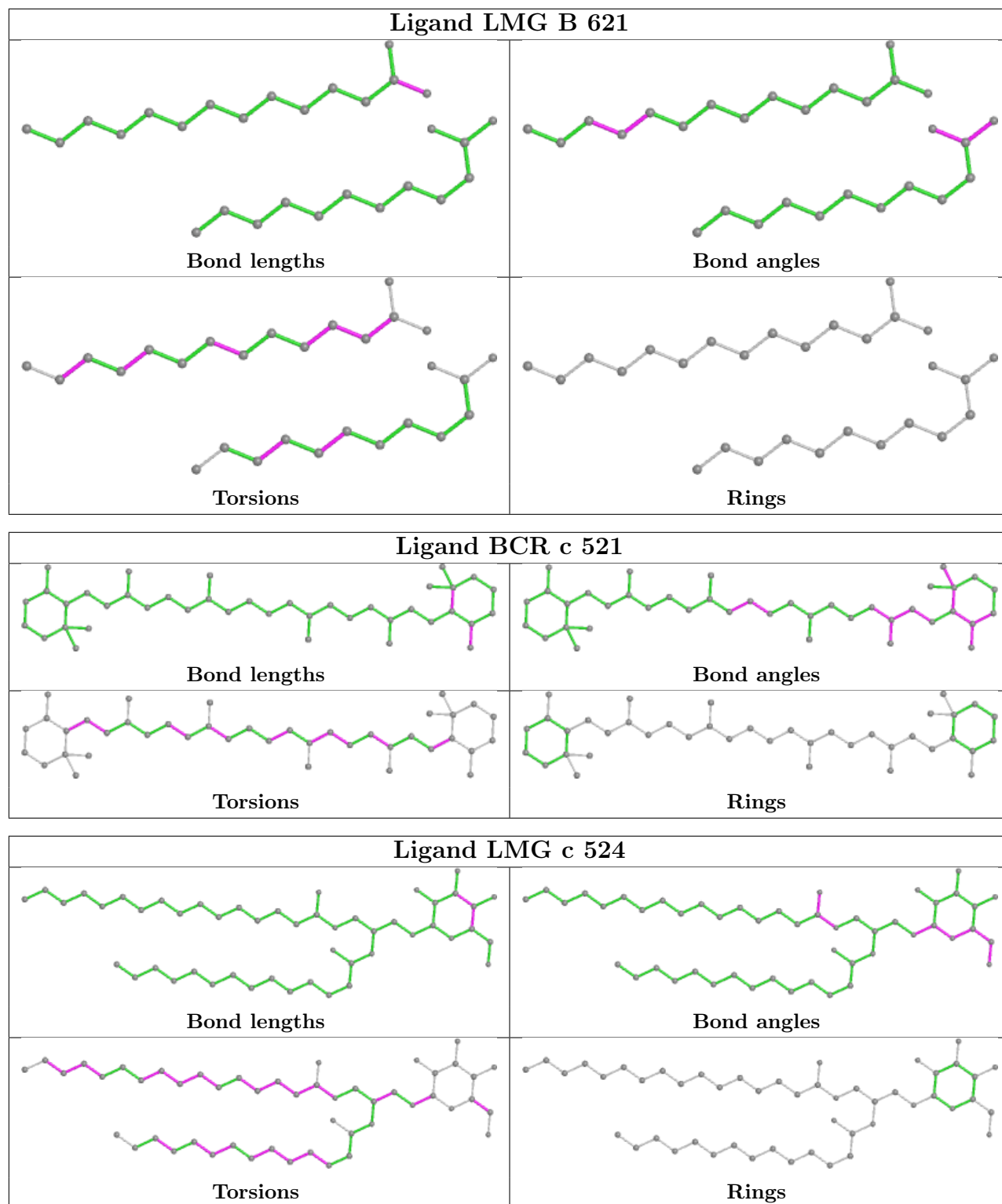


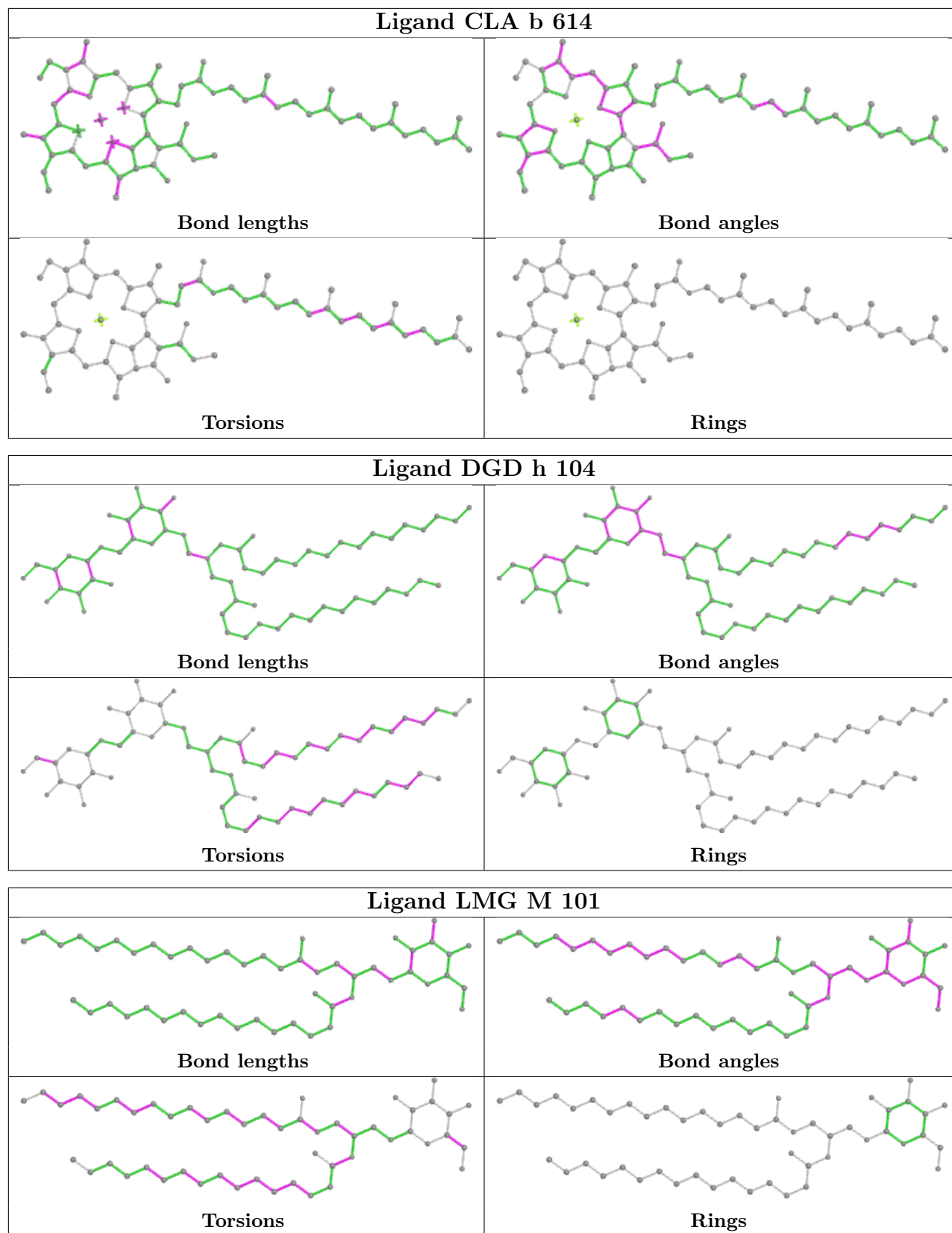


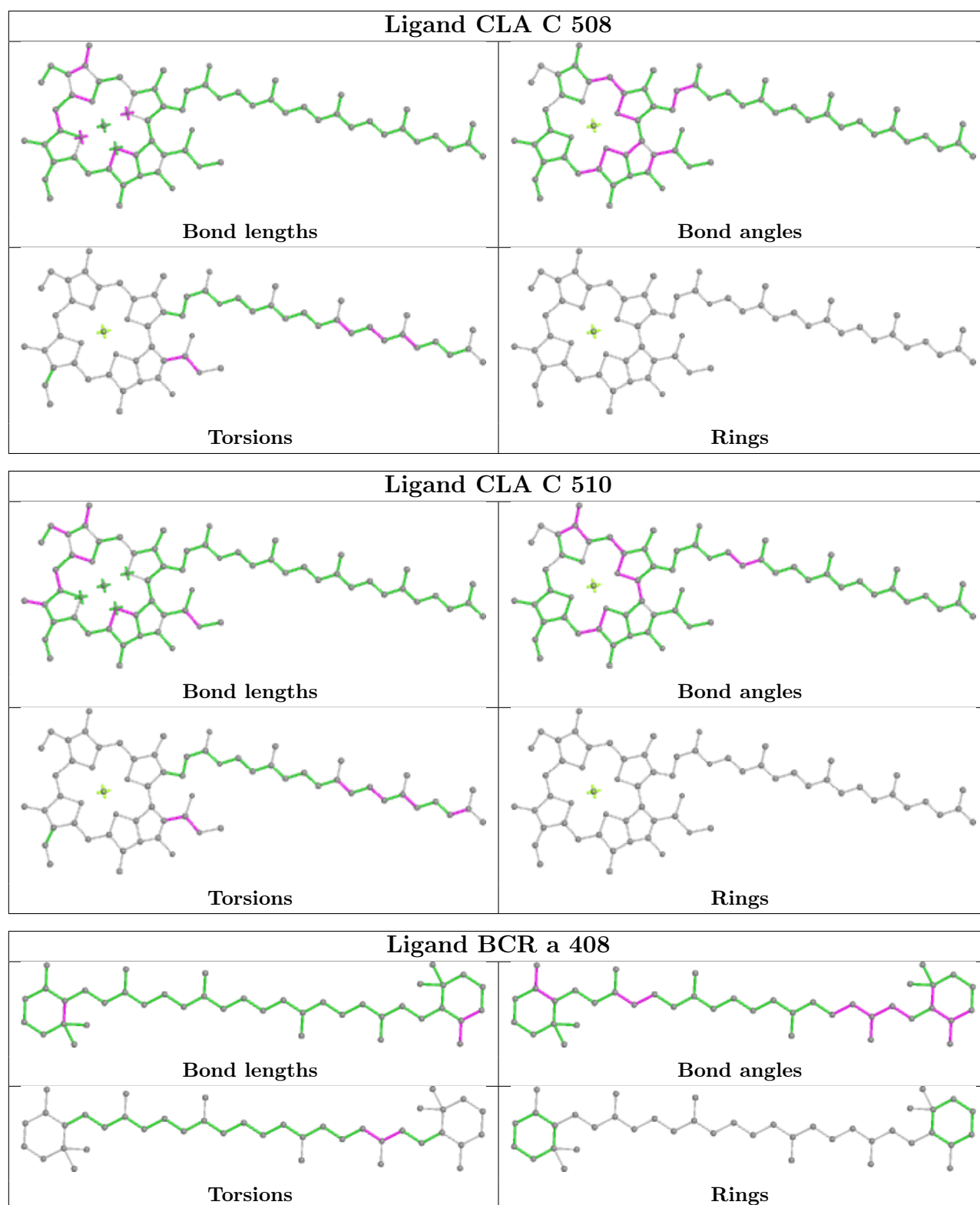


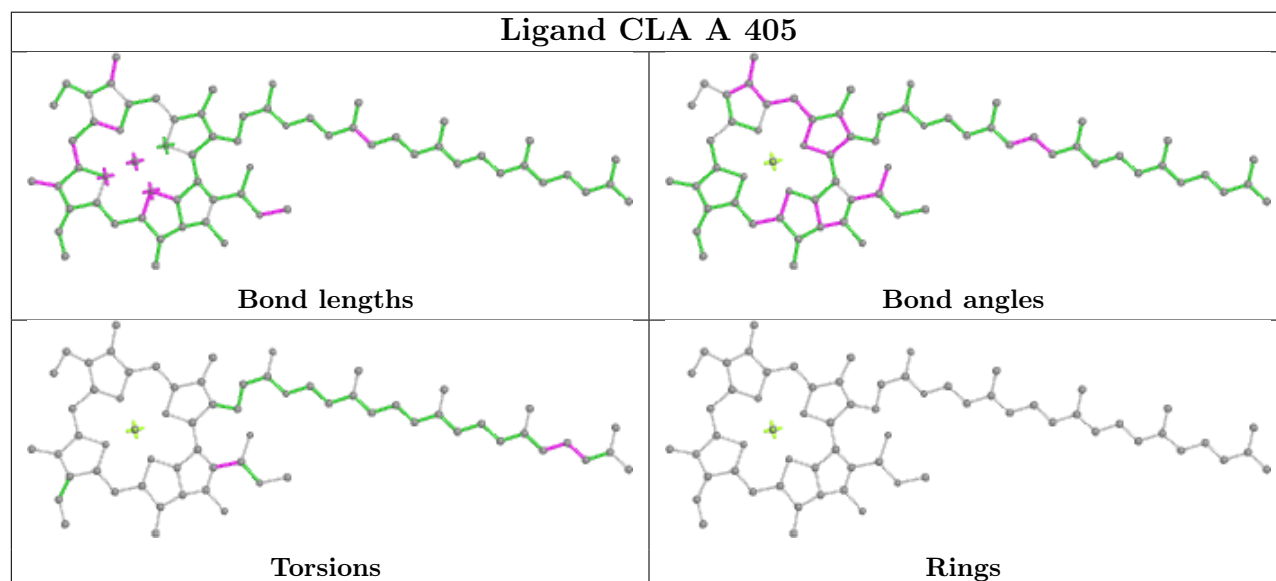
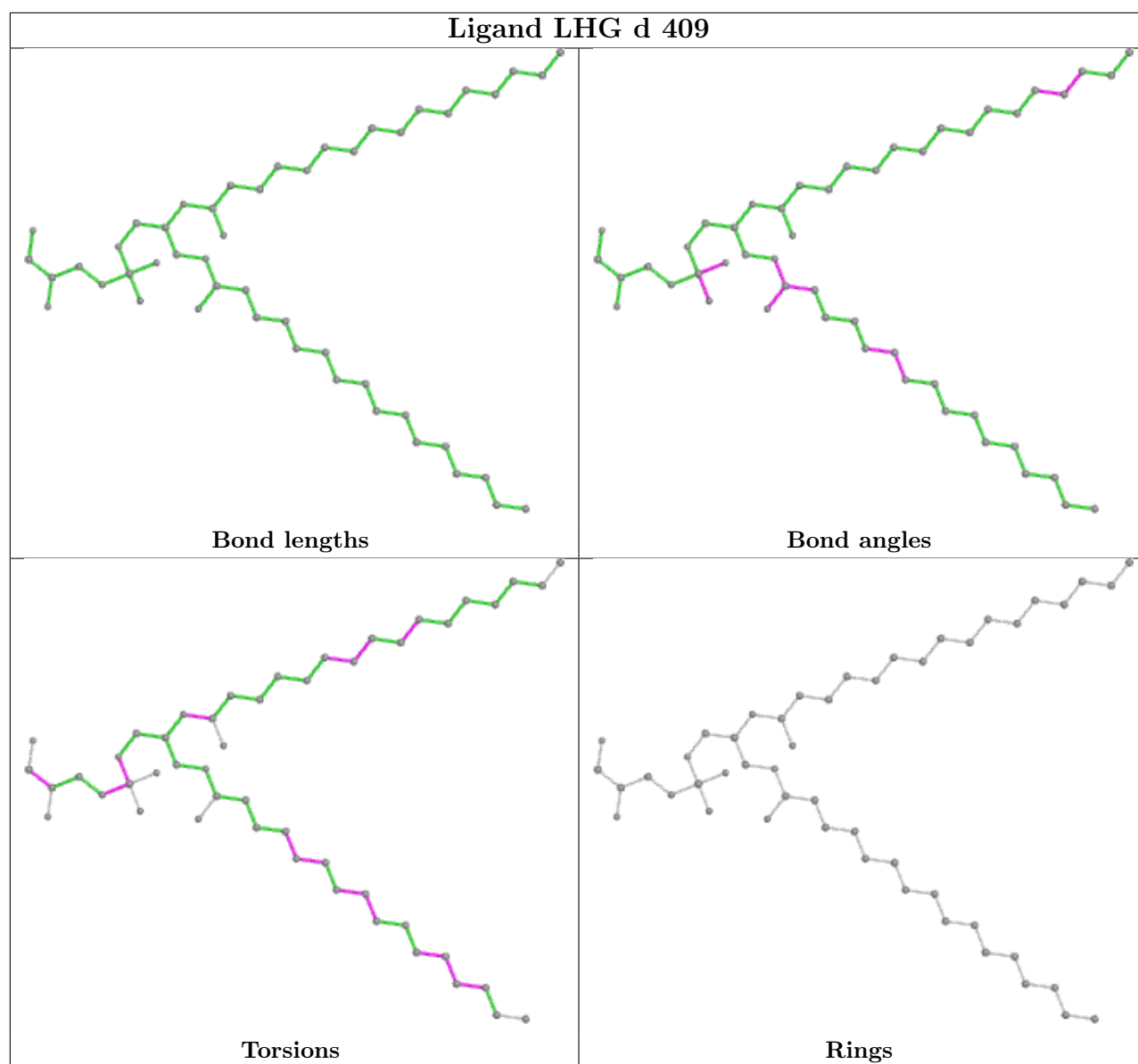


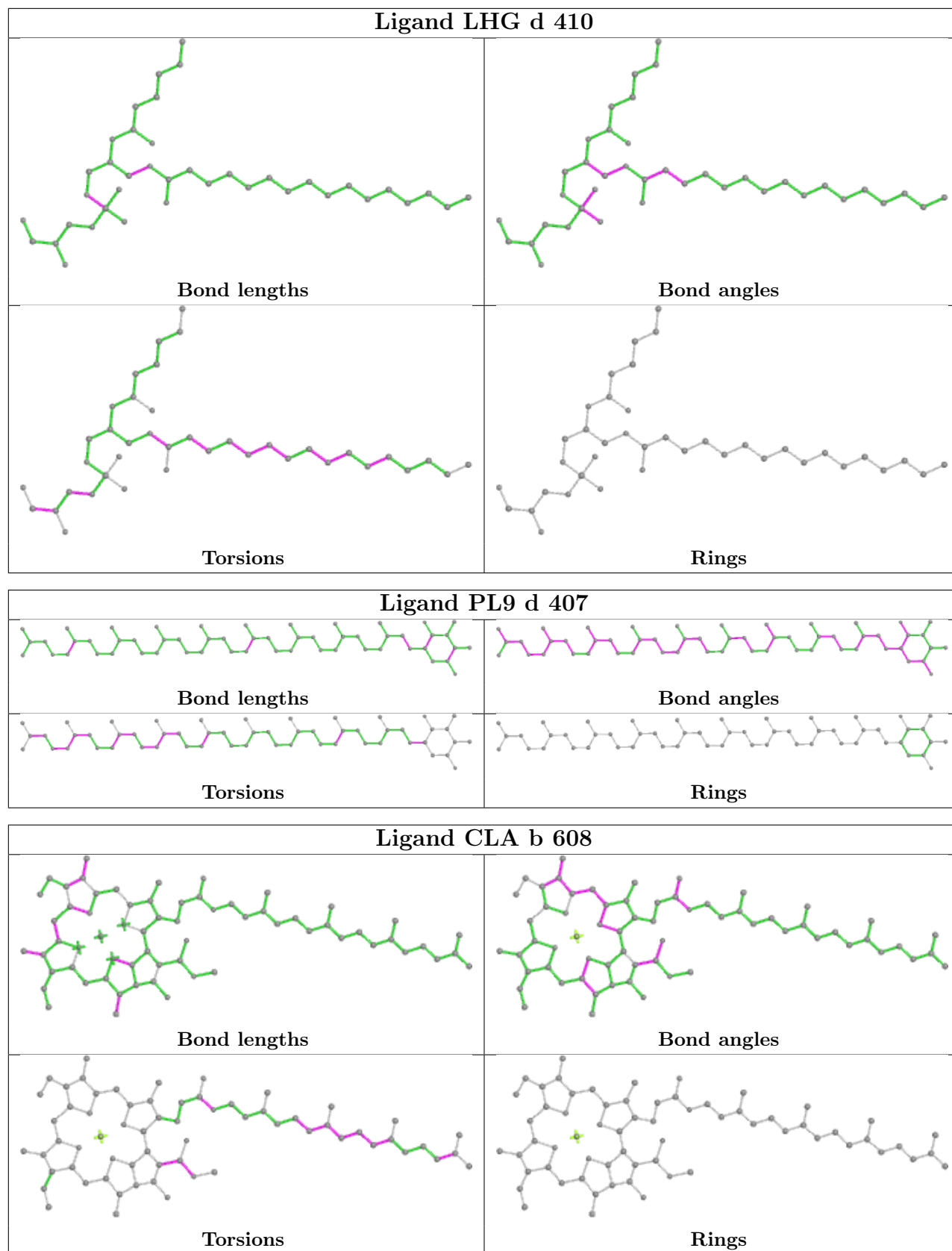


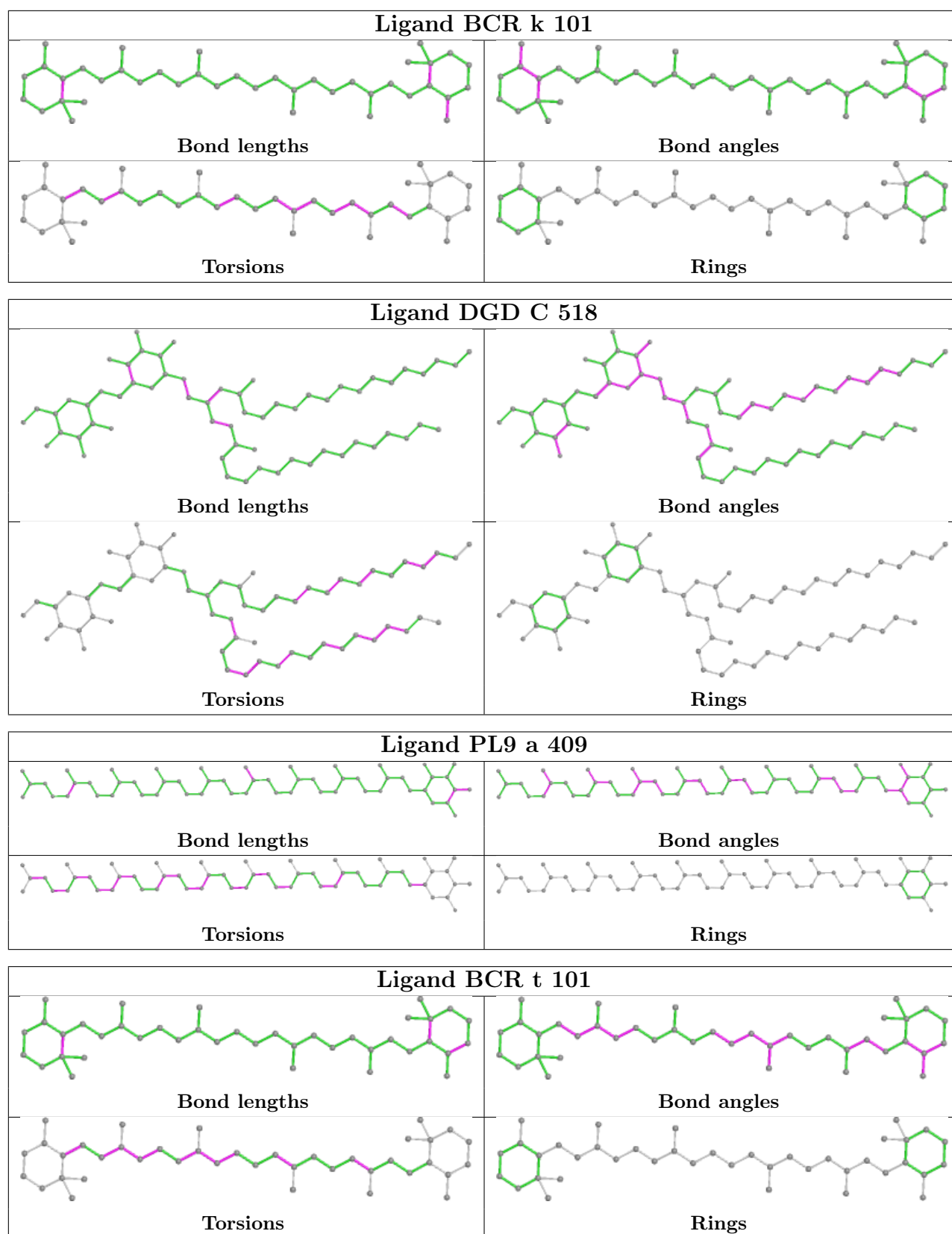


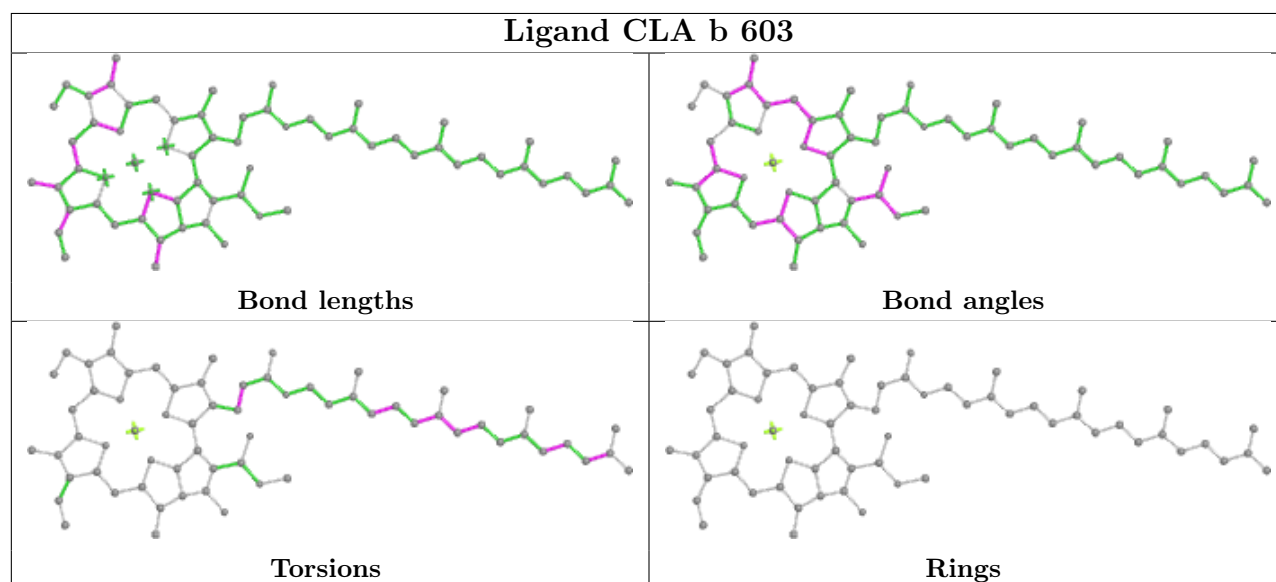
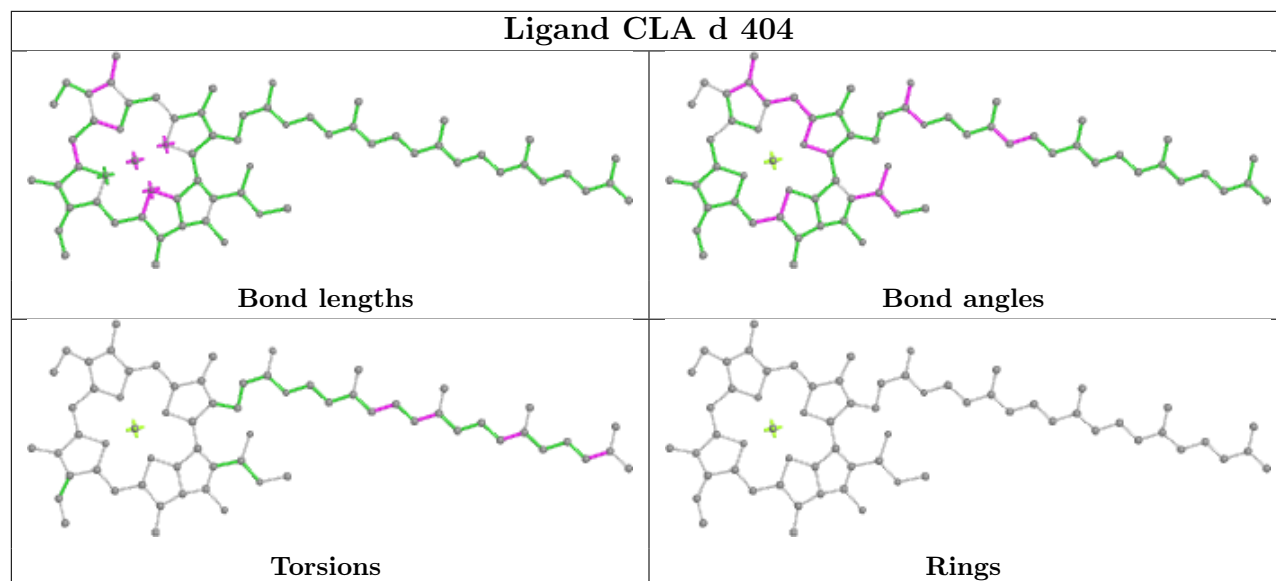
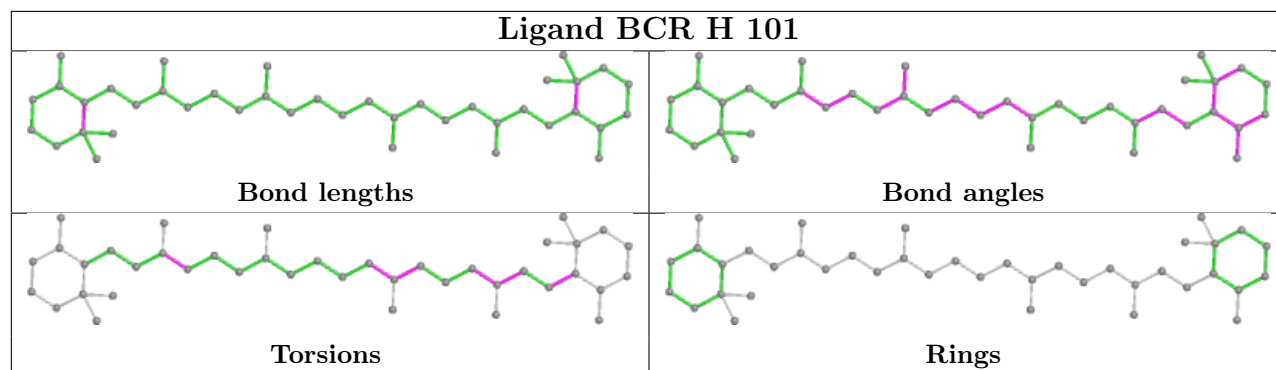


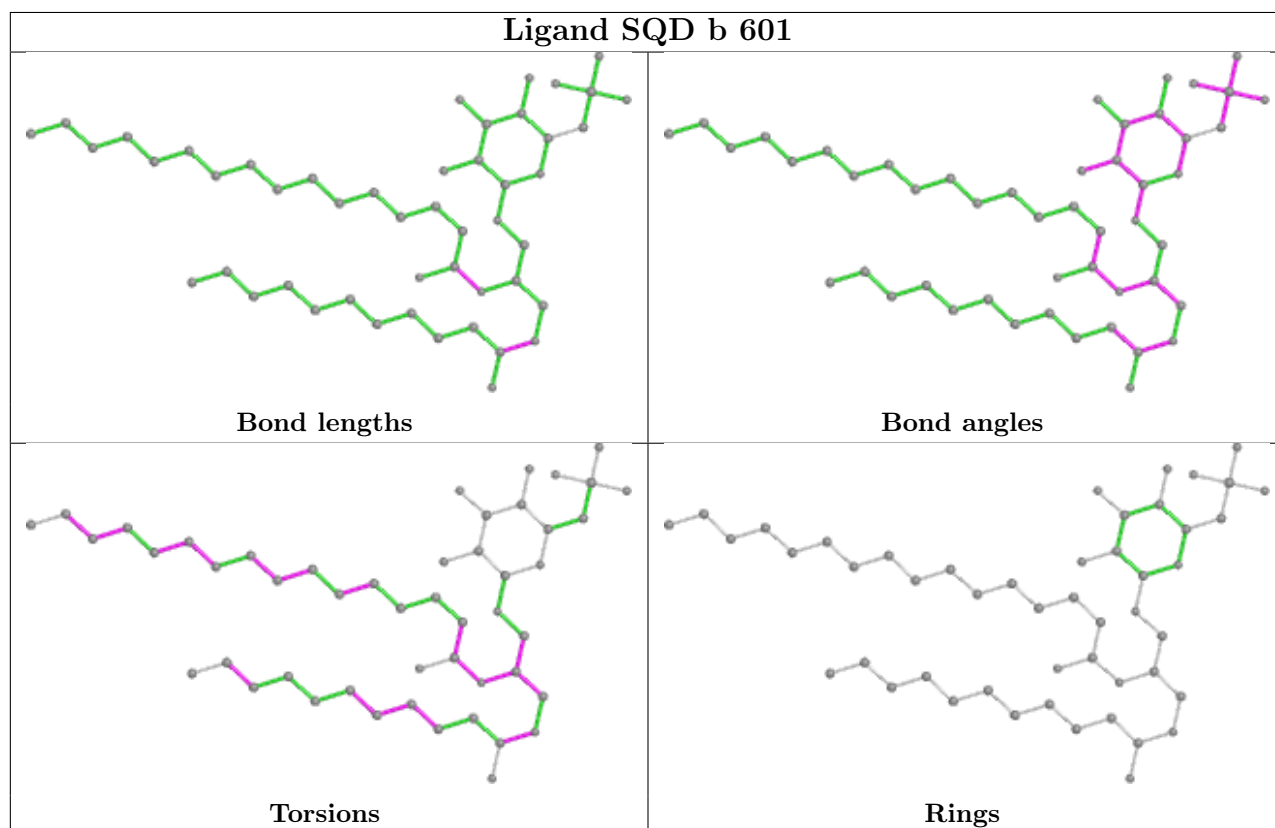
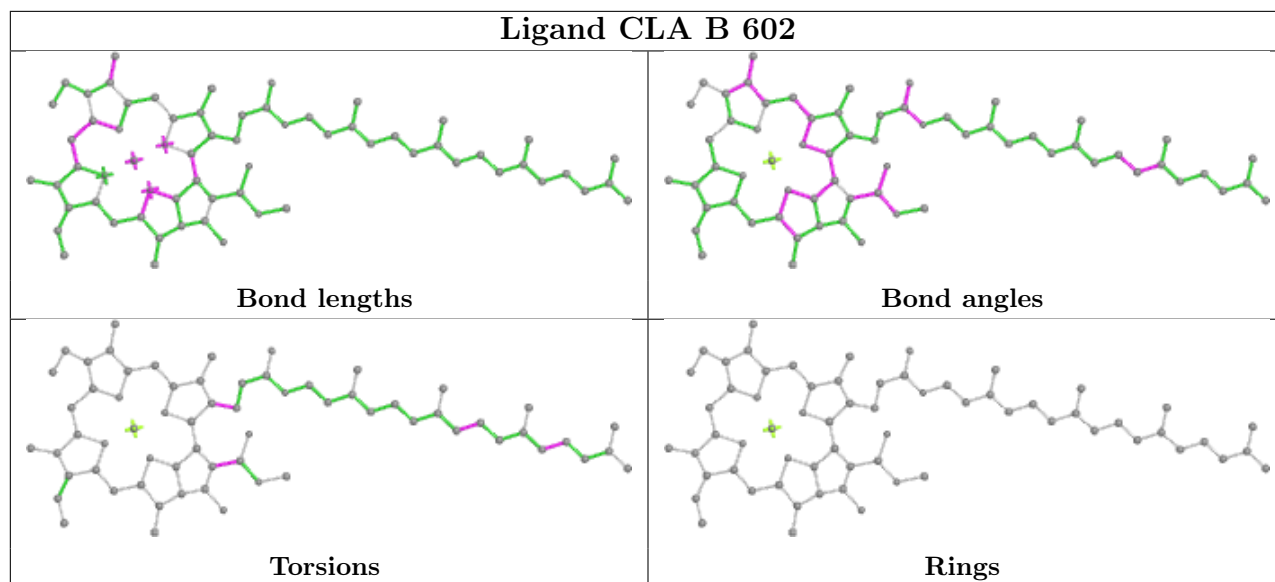


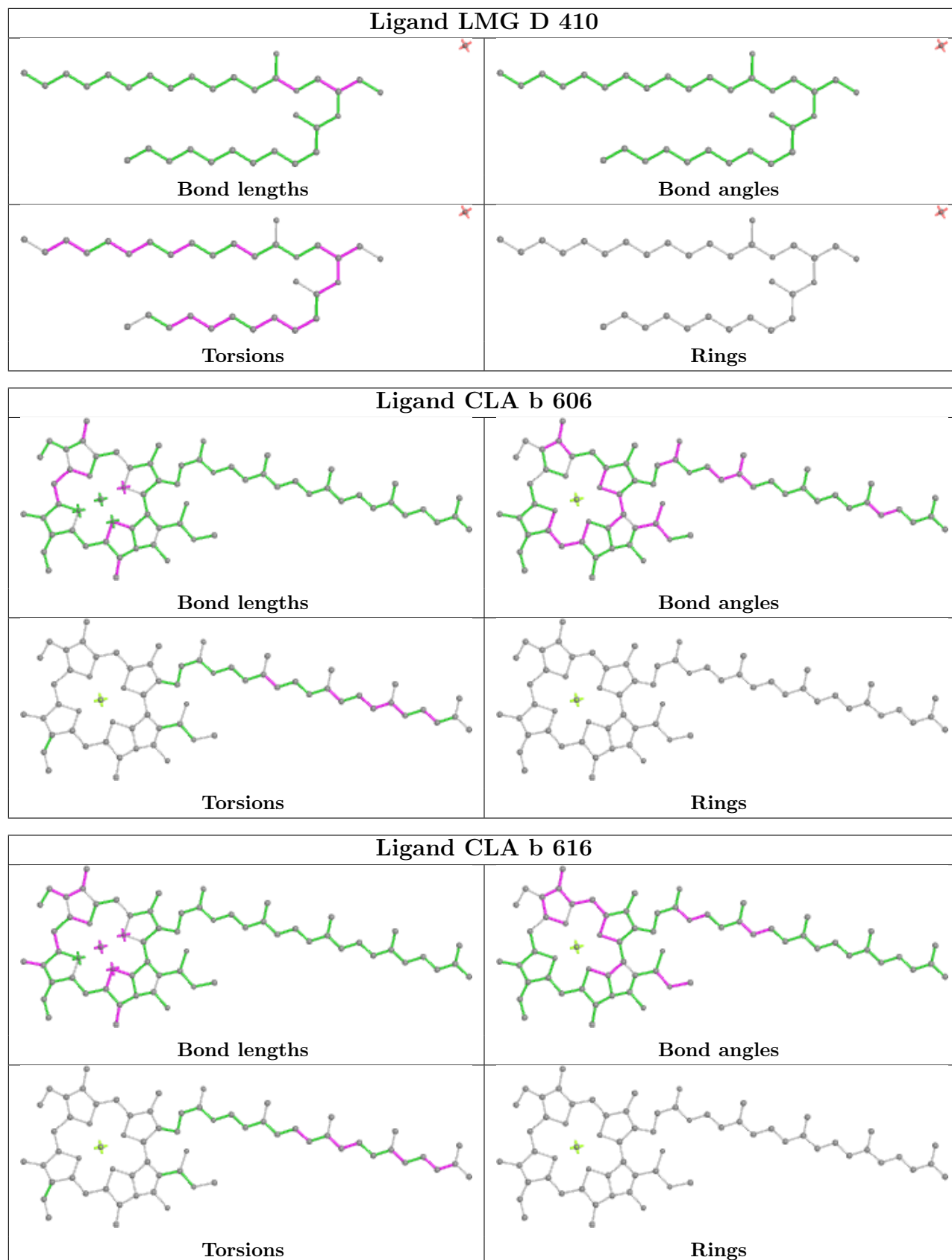


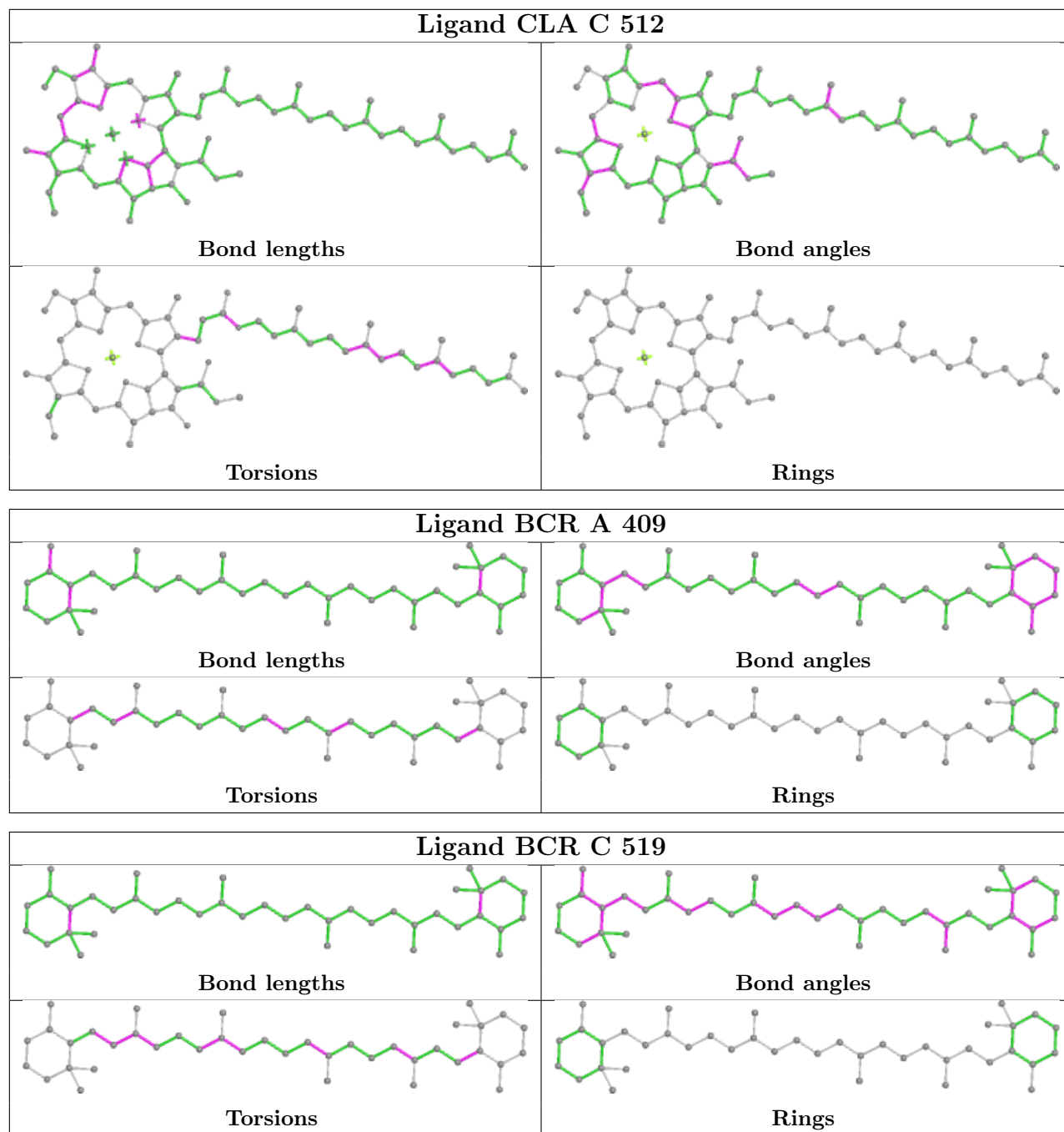


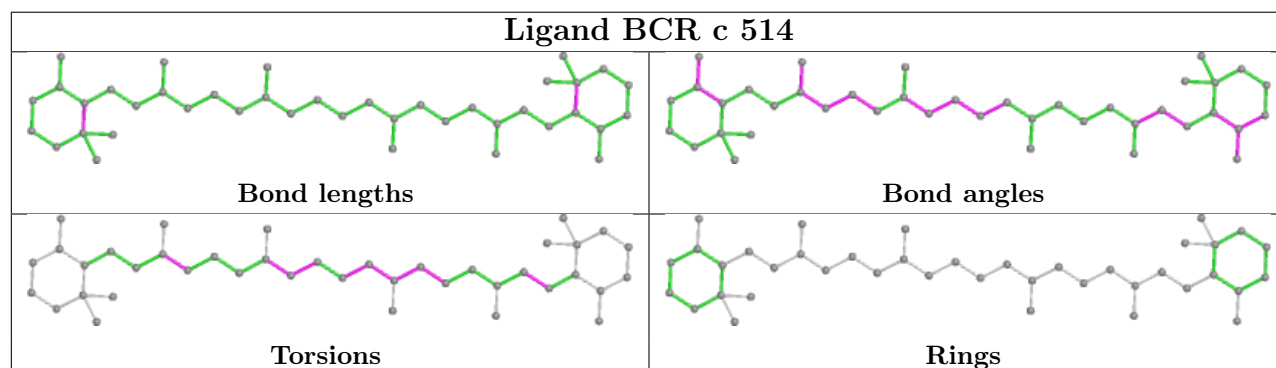
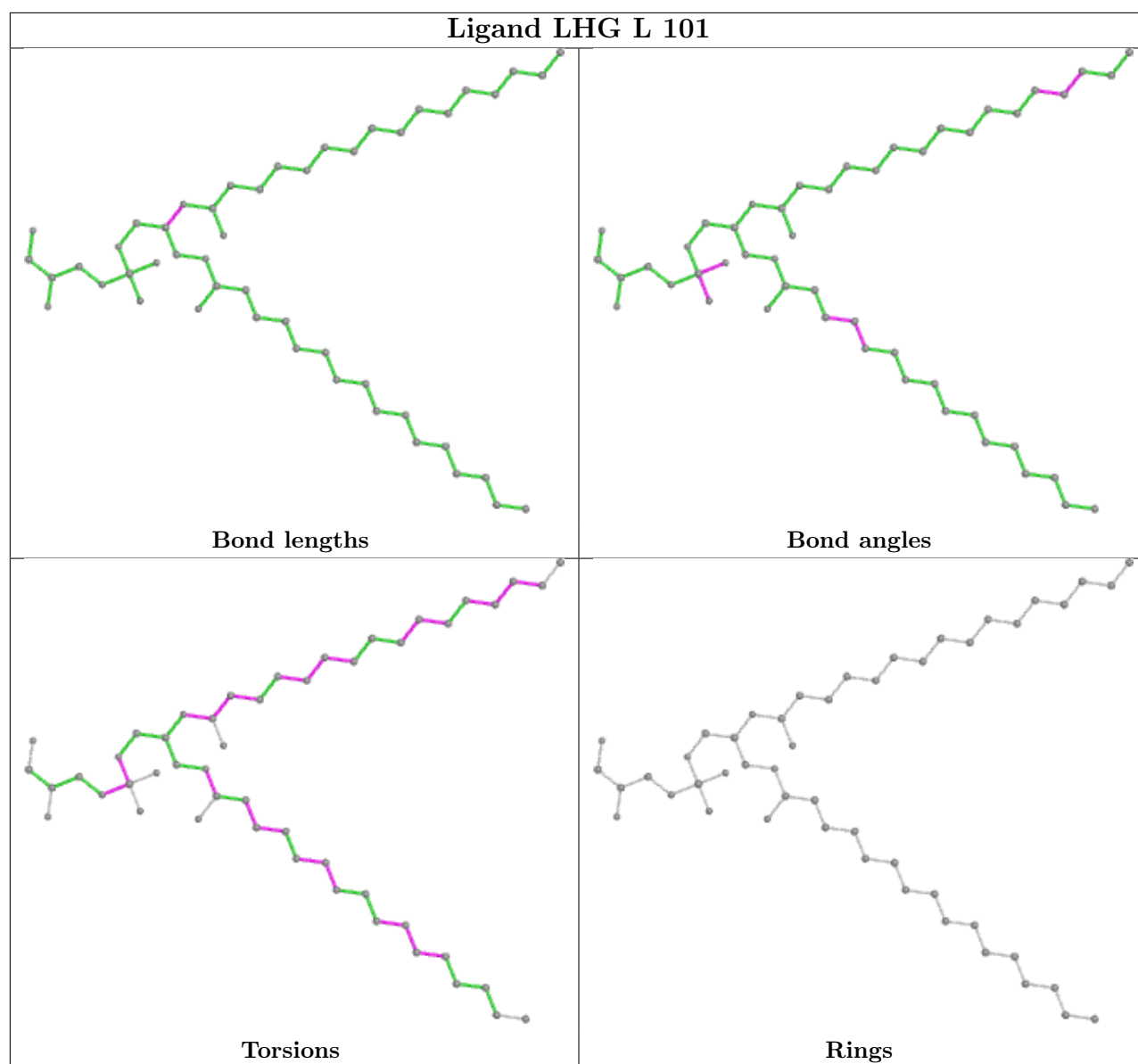


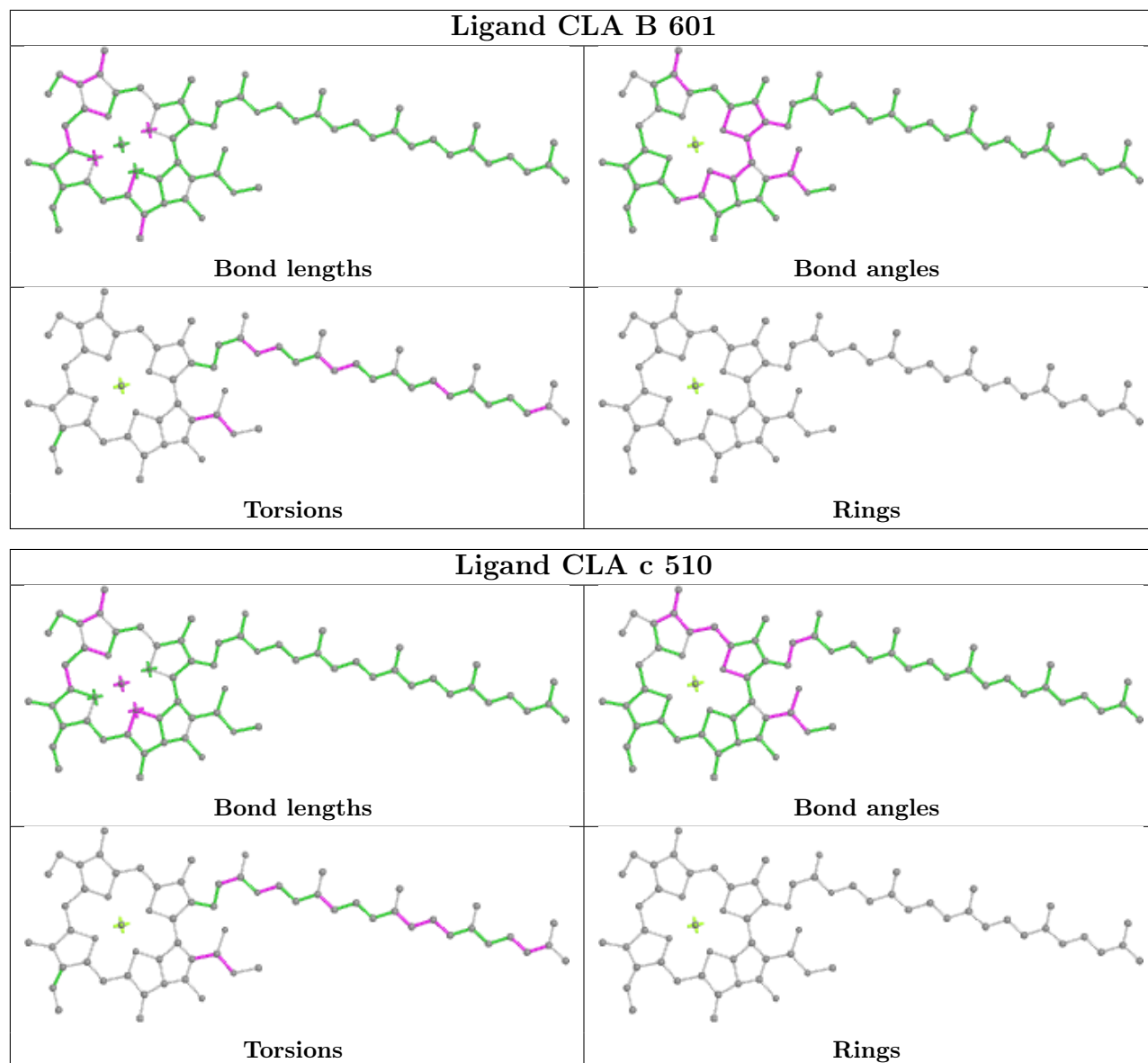


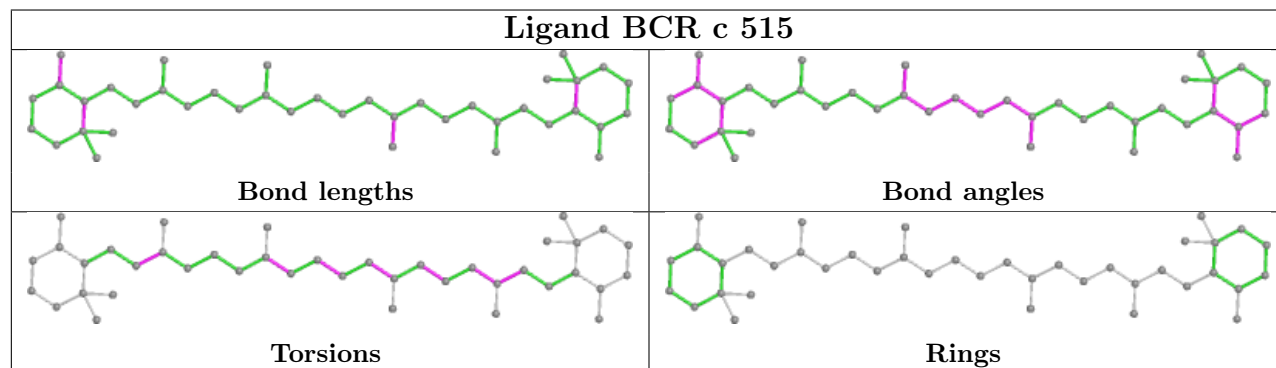
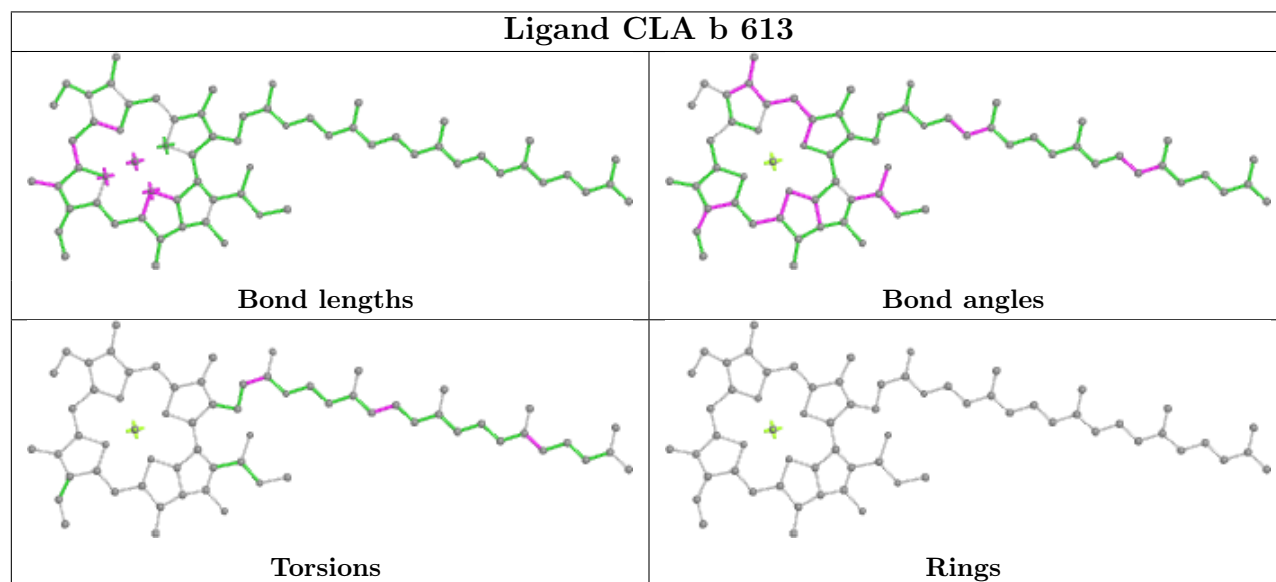
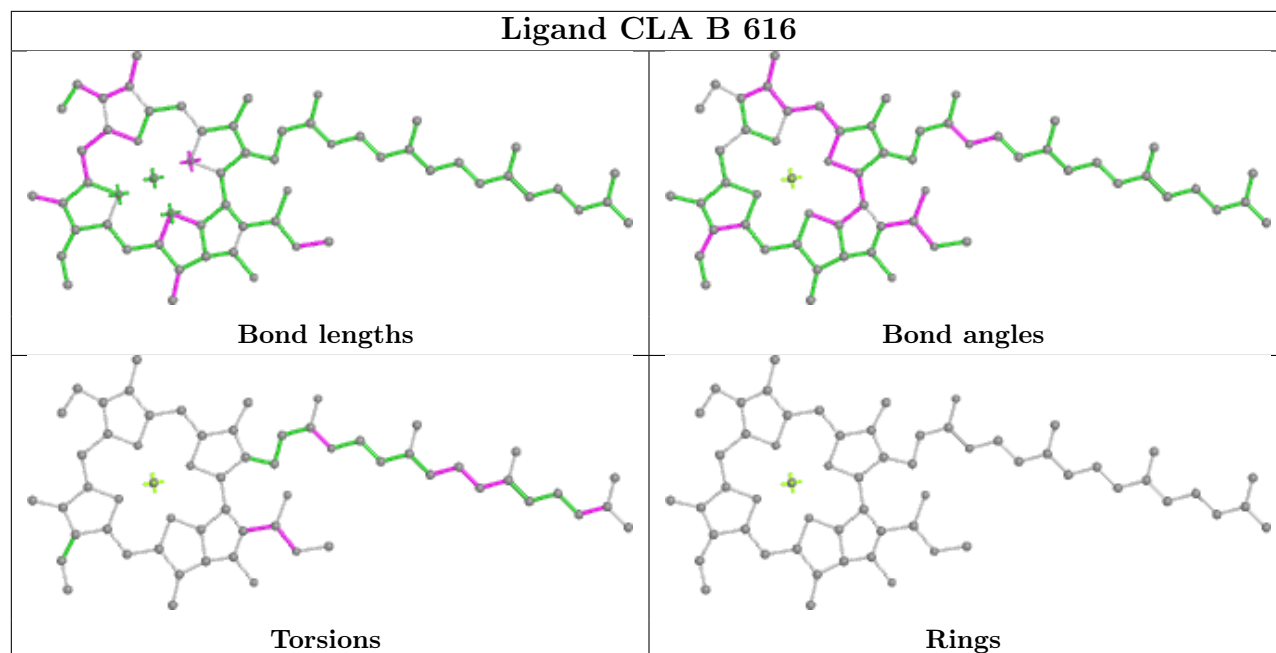


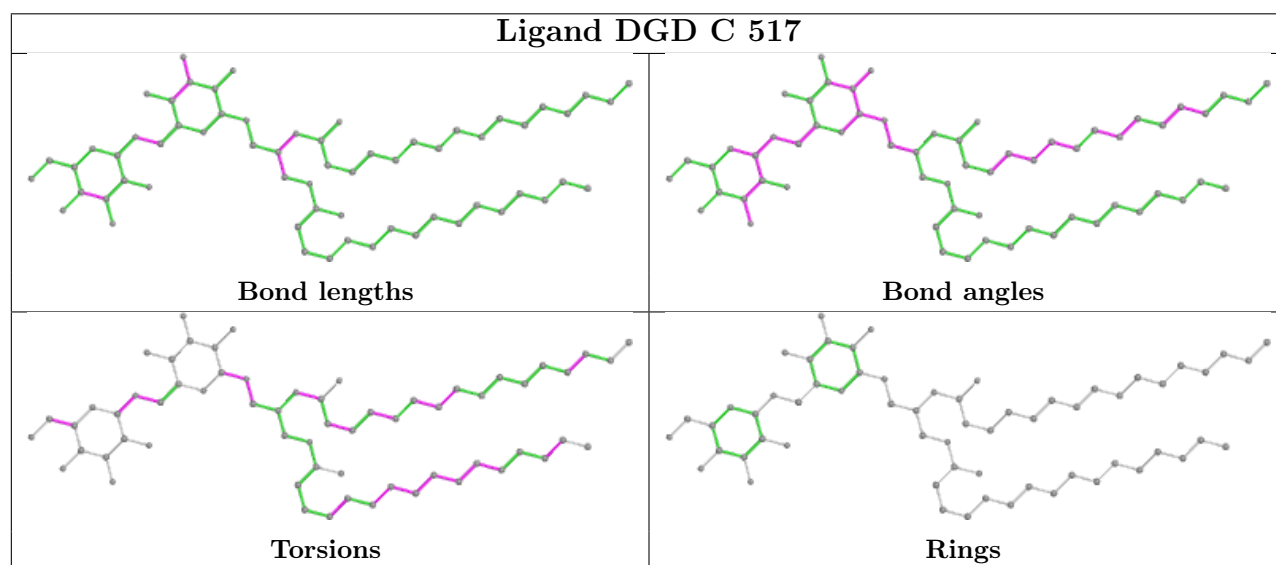
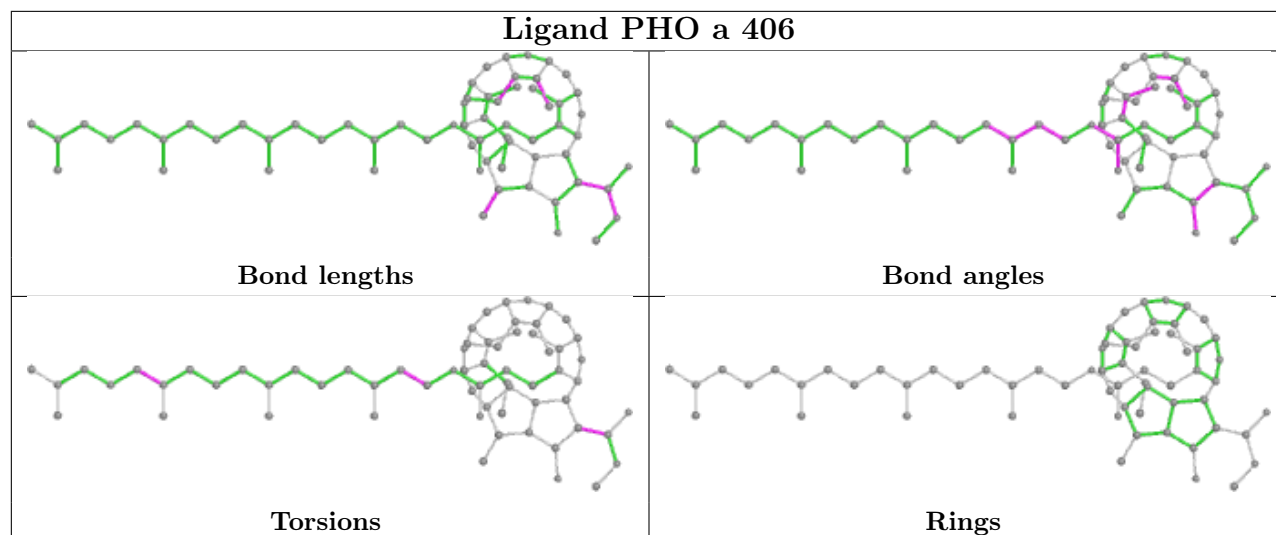


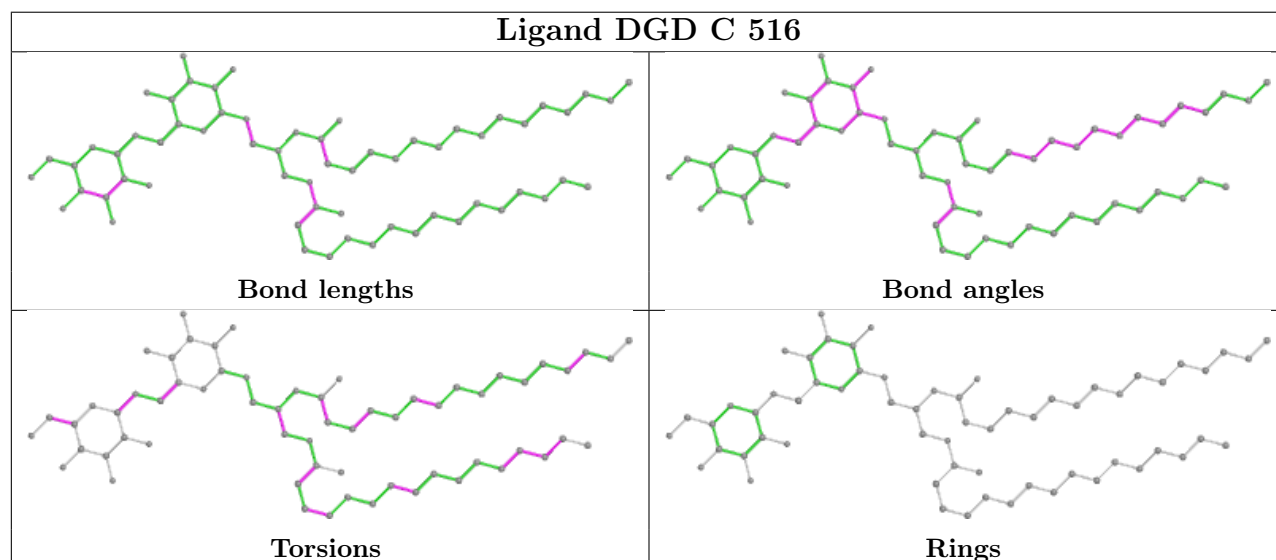
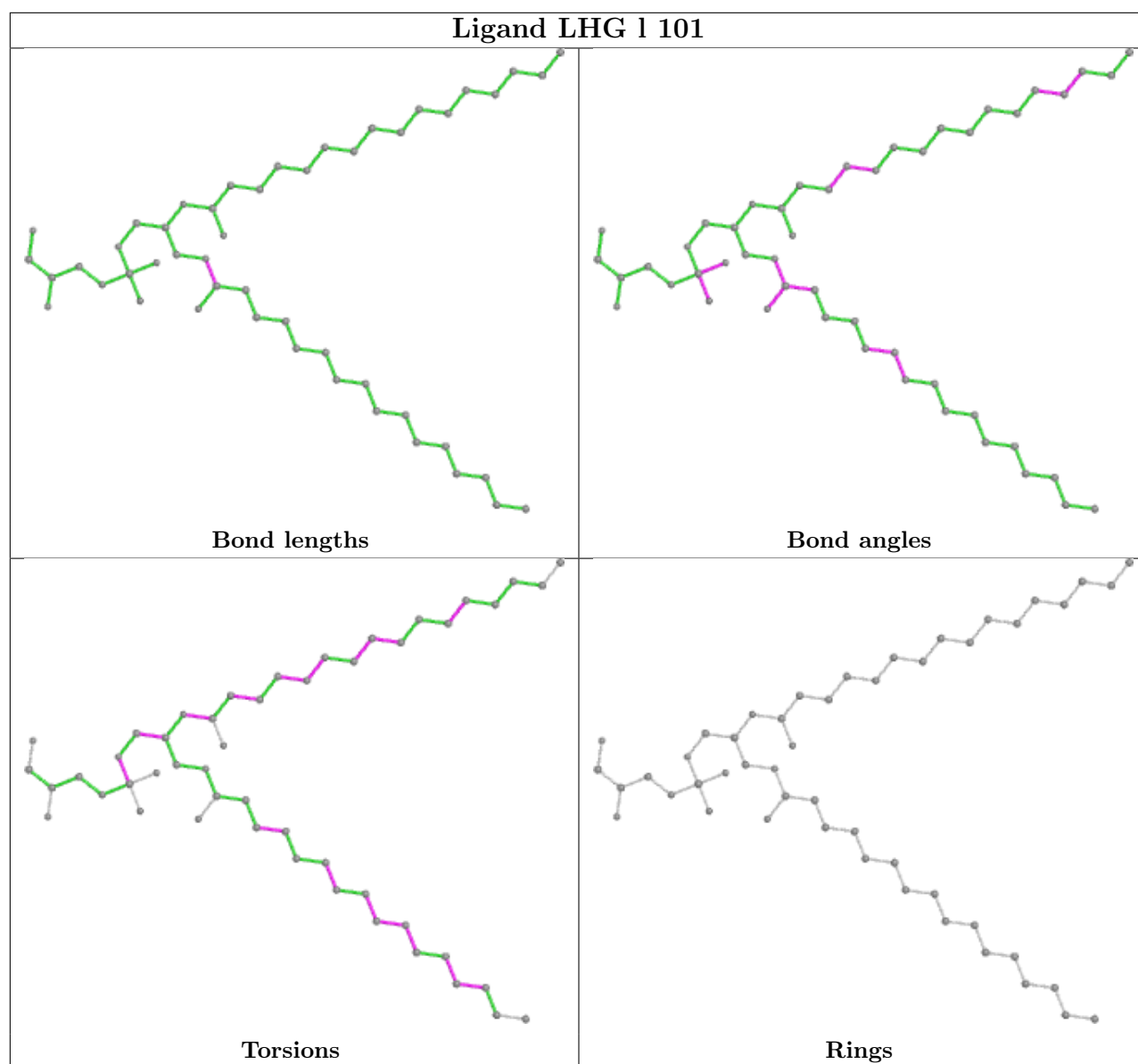


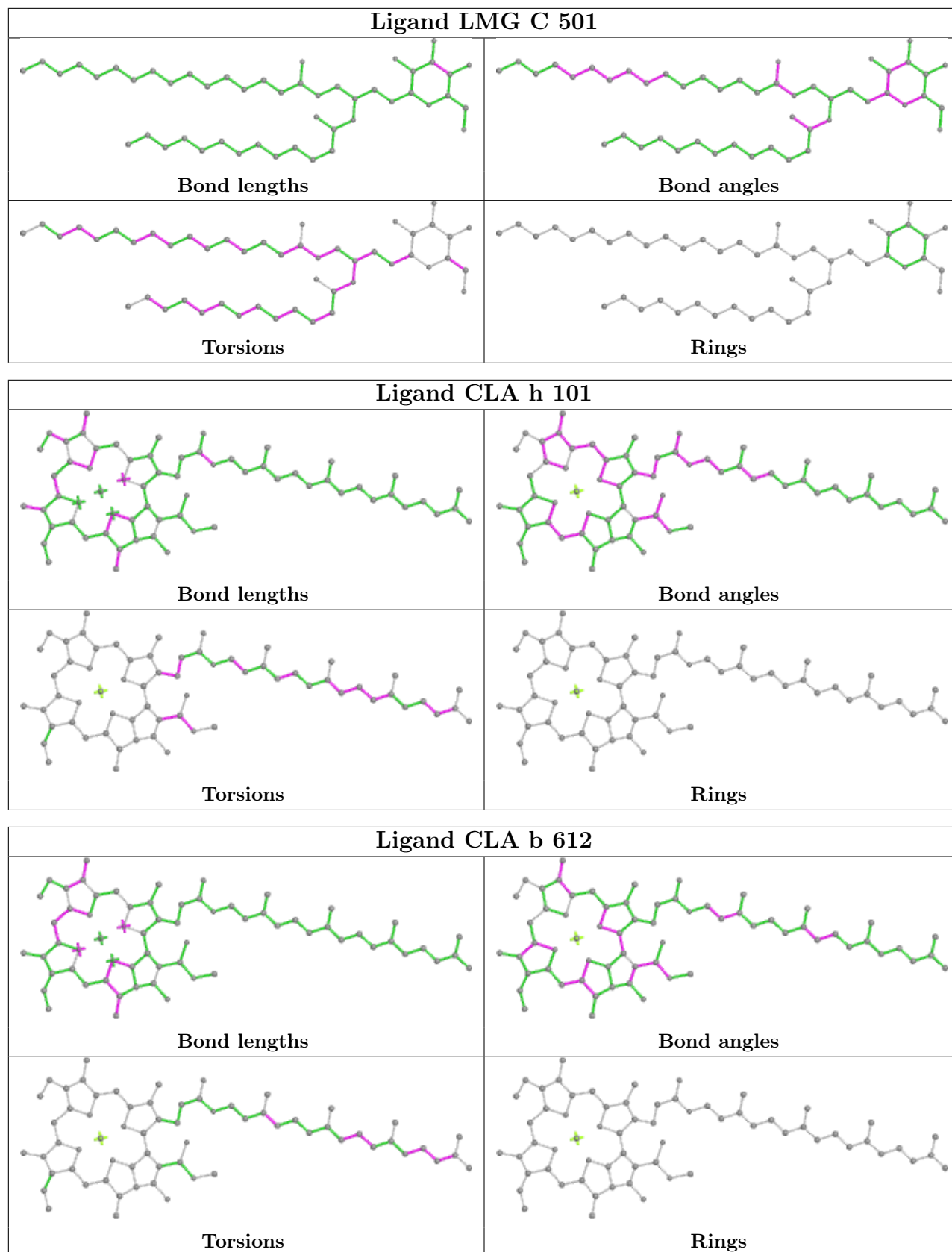


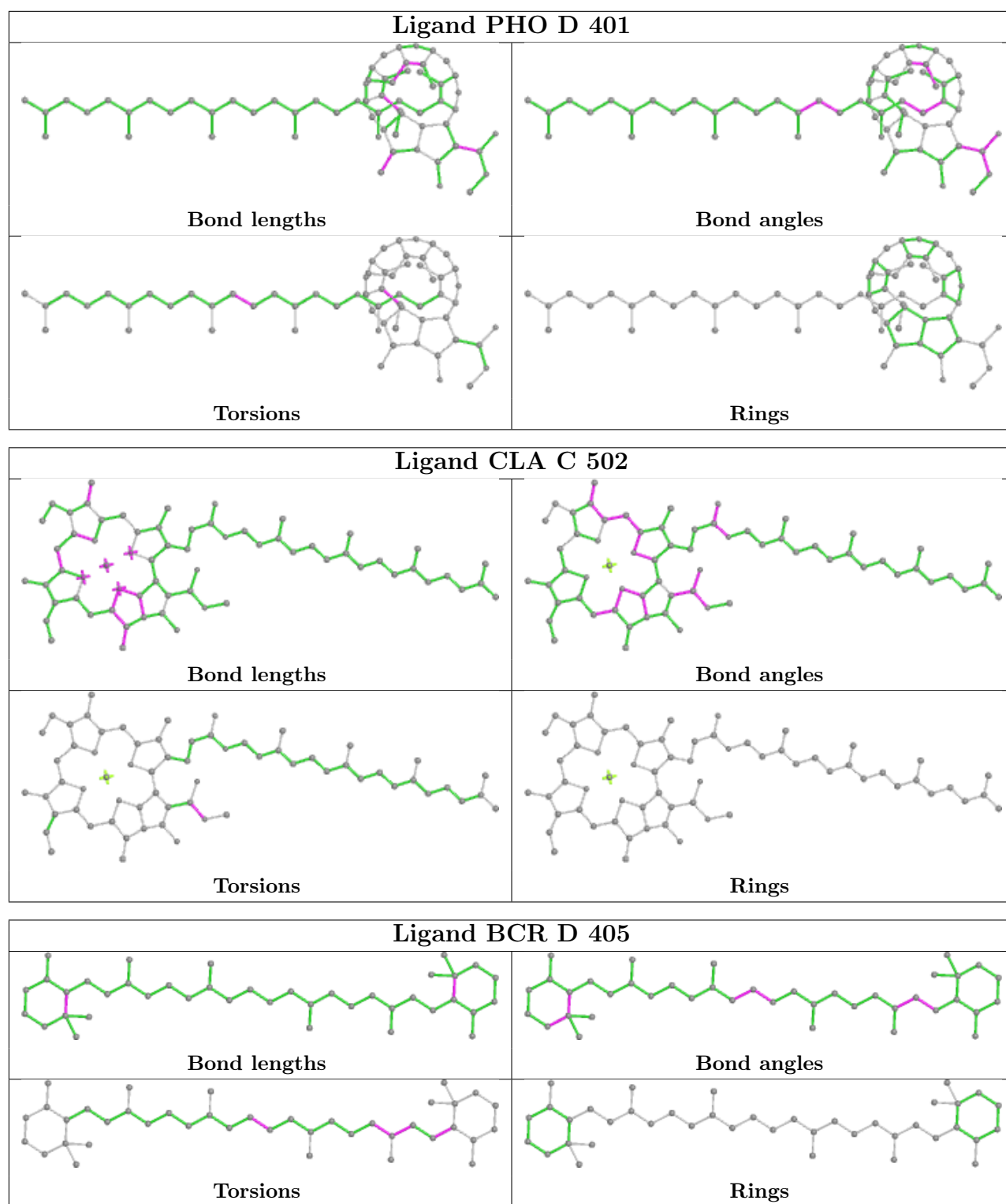


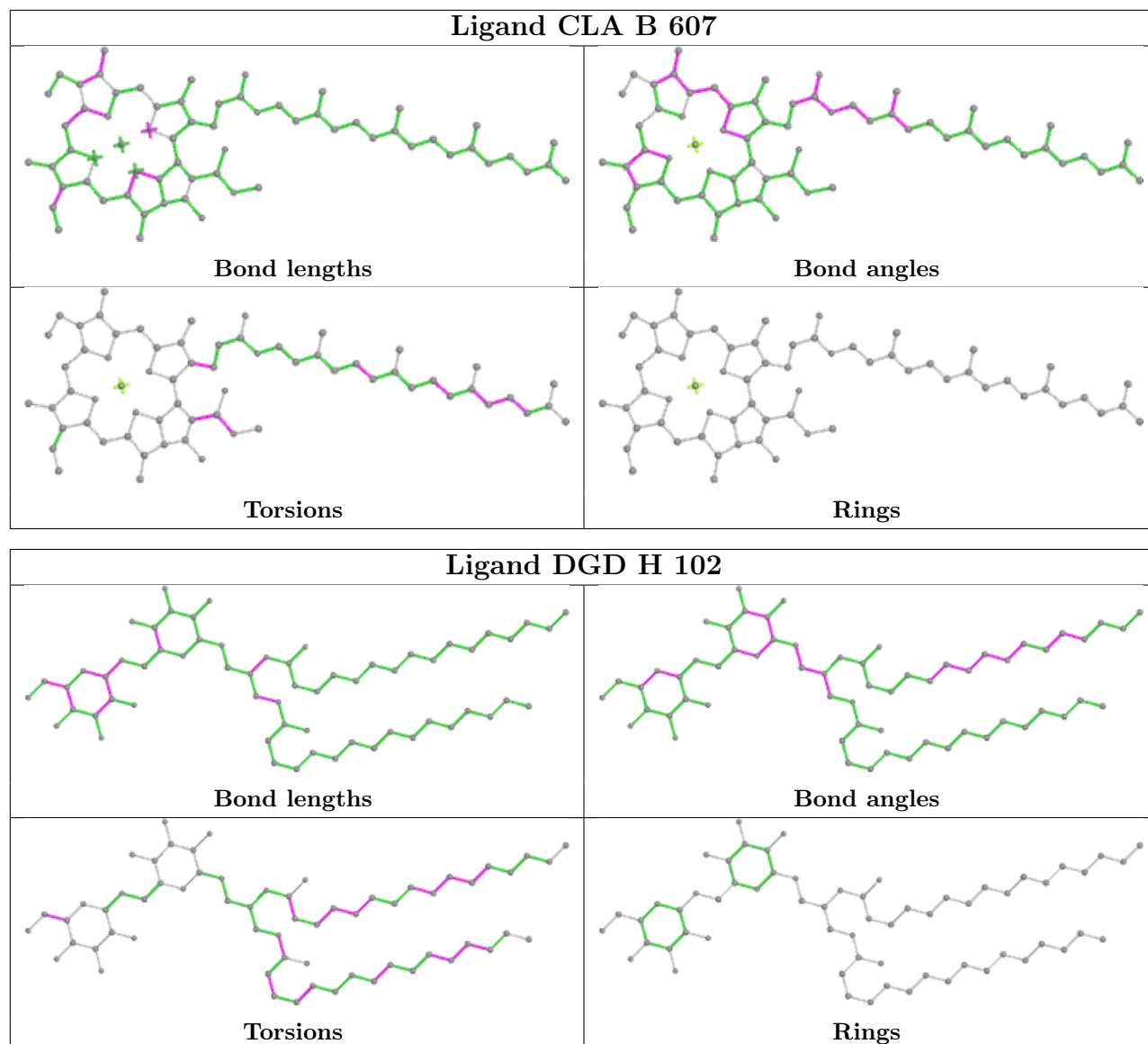


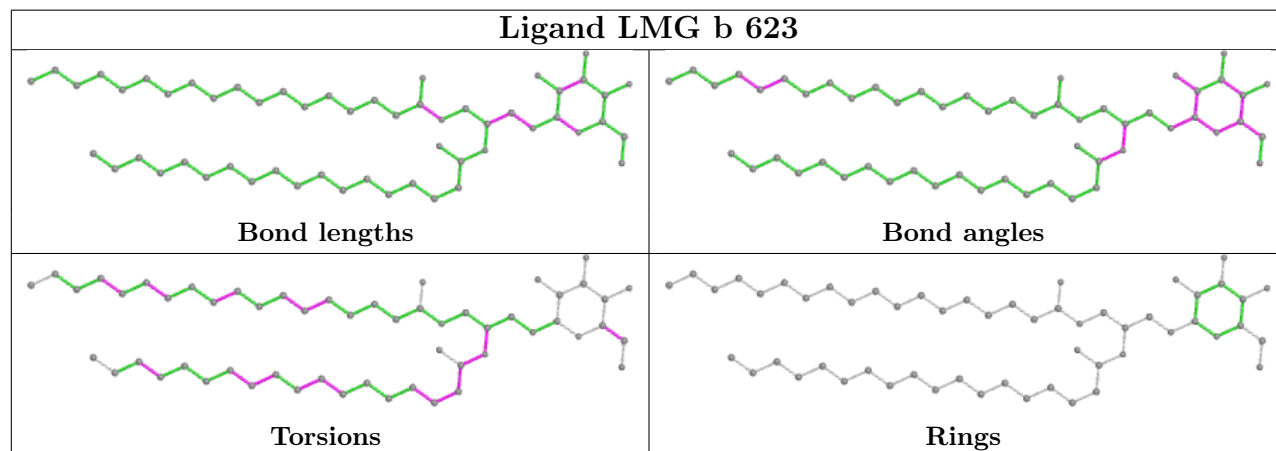
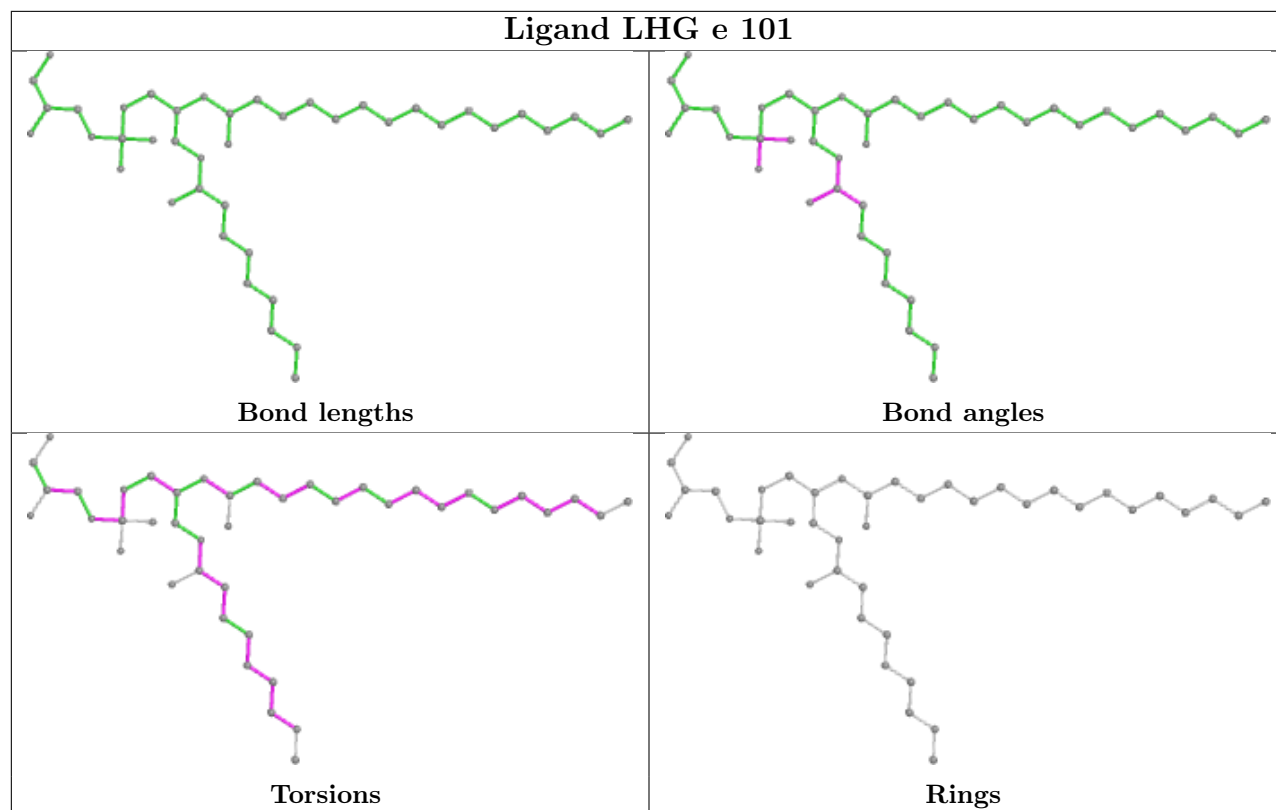


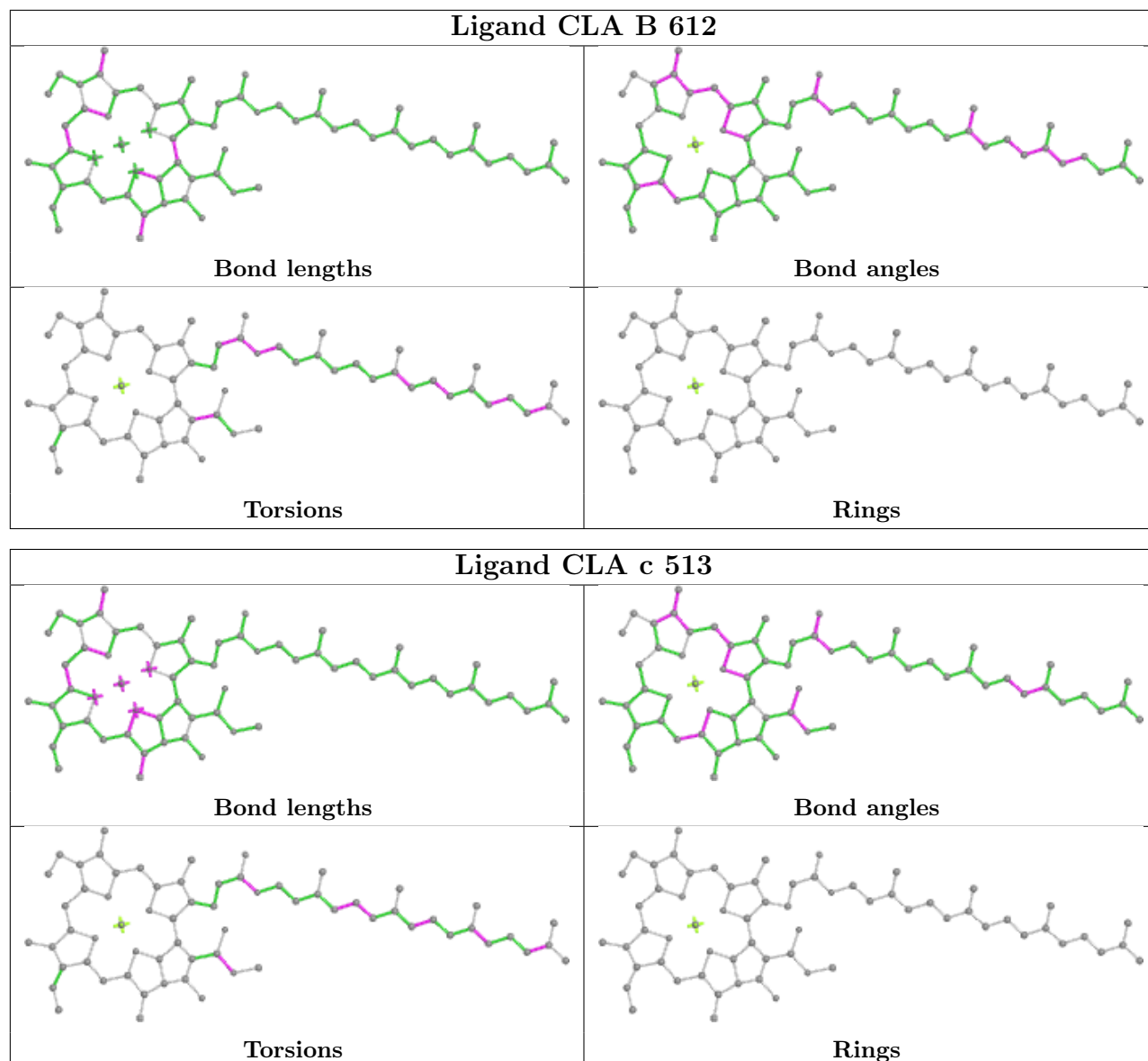


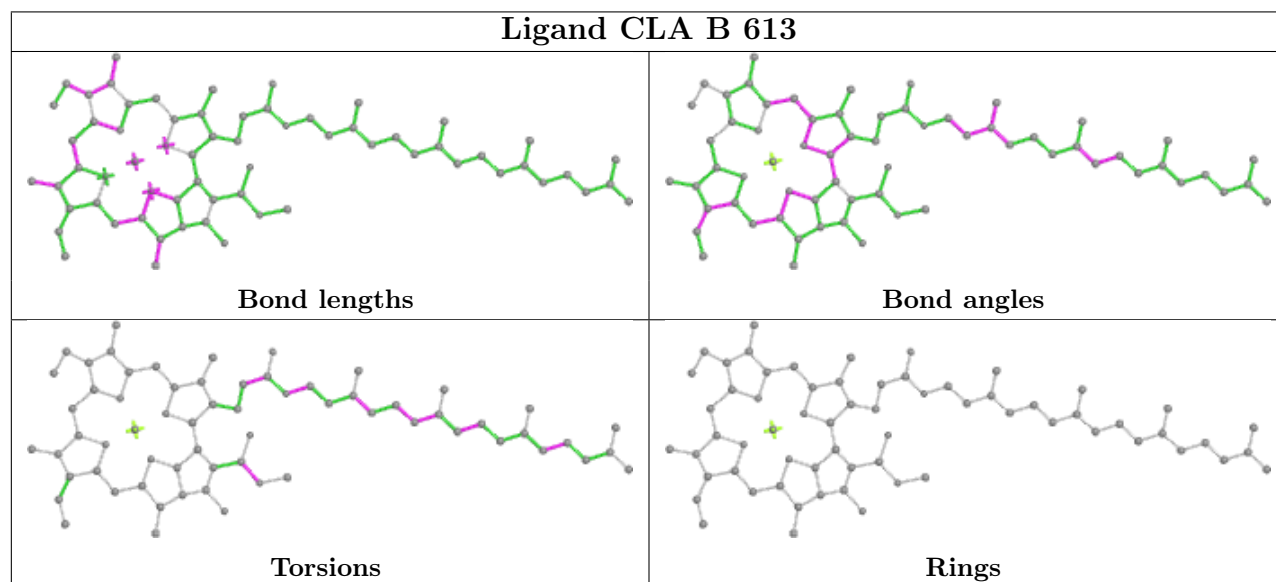
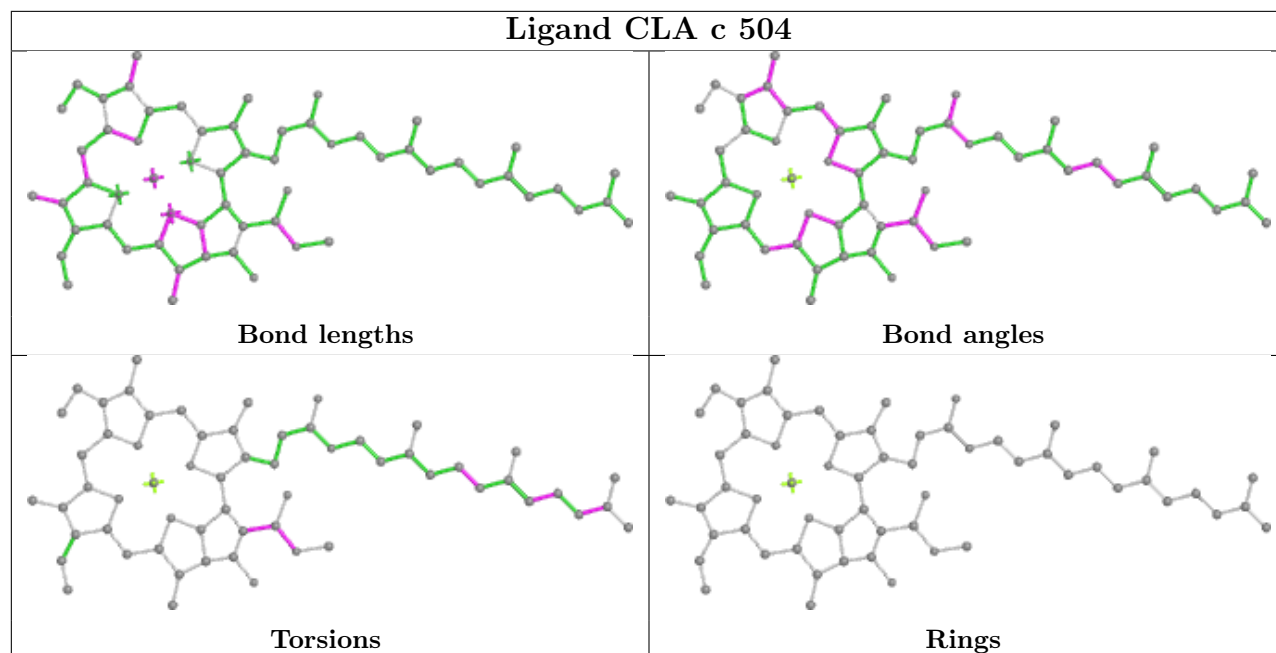


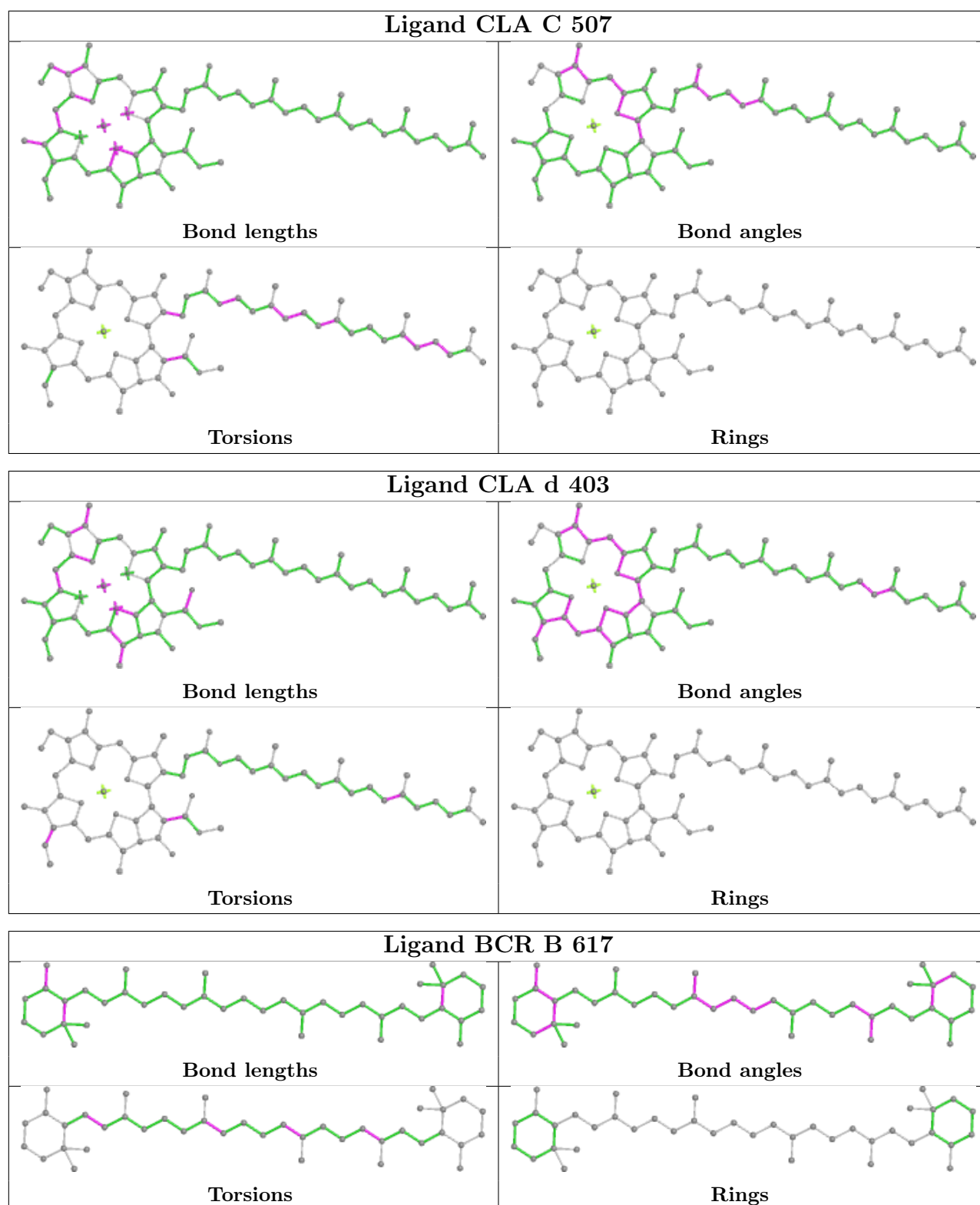


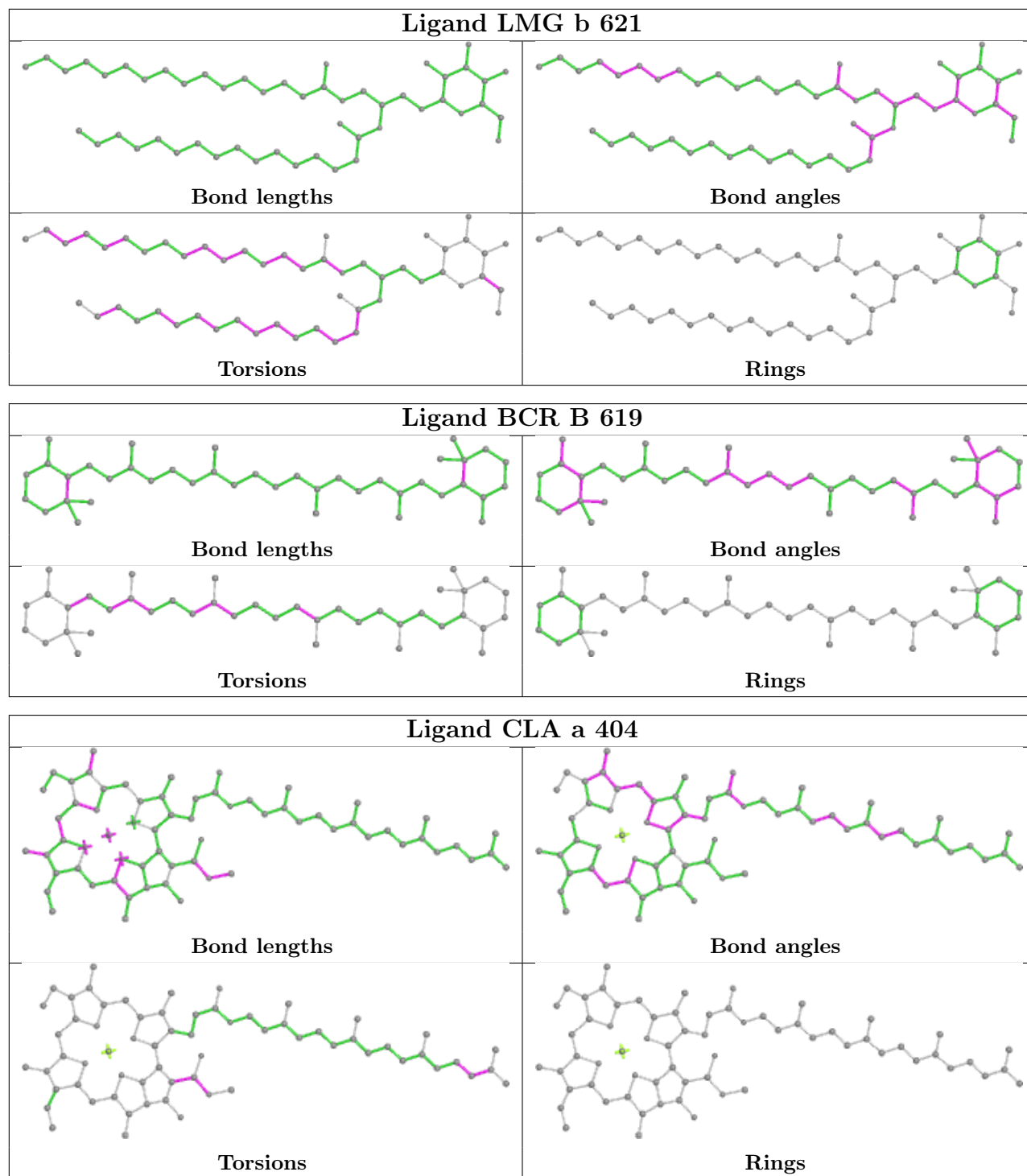


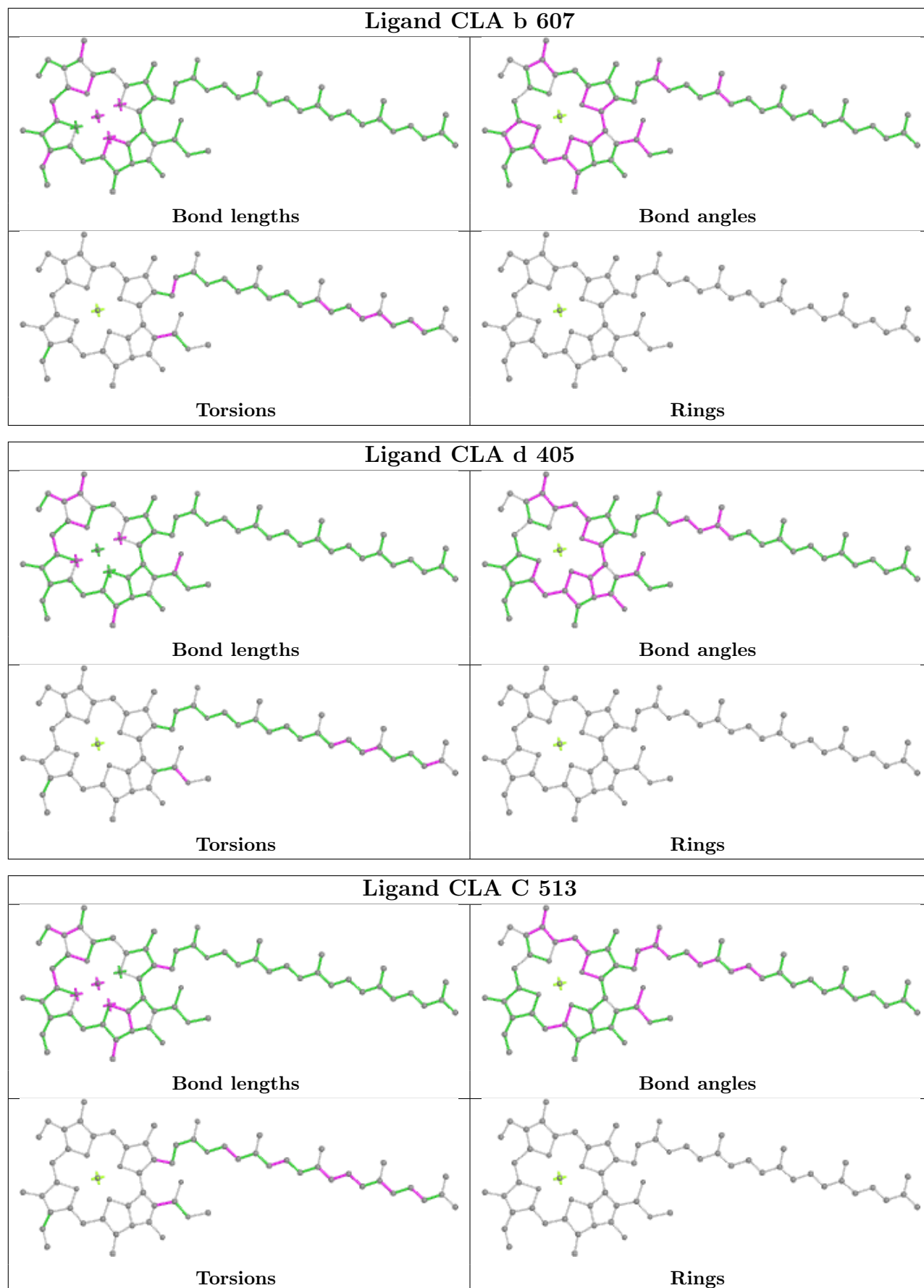


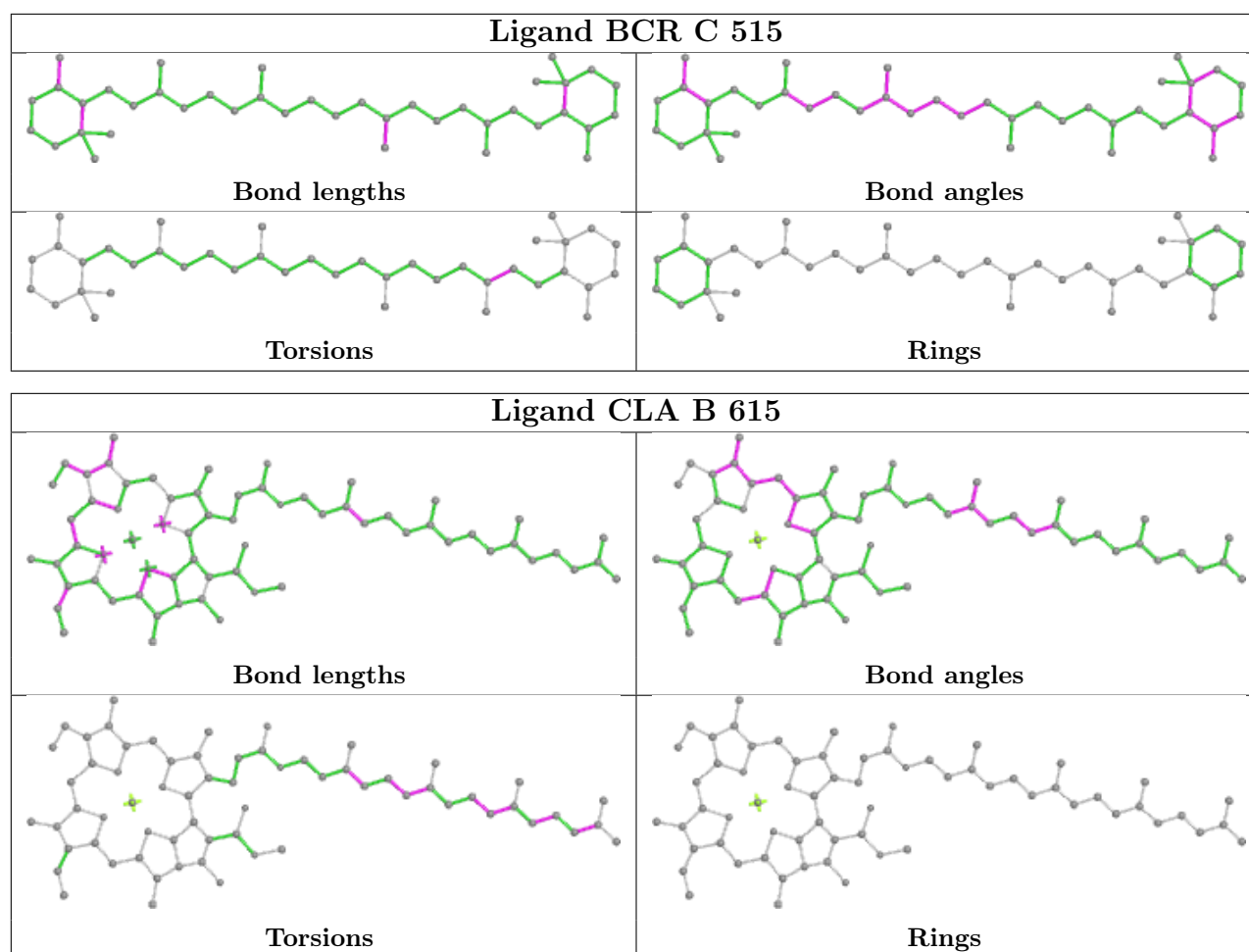












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	468:SER	C	469:MET	N	1.17

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/334 (100%)	-0.42	3 (0%) 84 86	20, 28, 47, 75	0
1	a	334/334 (100%)	-0.42	1 (0%) 94 94	22, 30, 59, 81	0
2	B	505/505 (100%)	-0.36	5 (0%) 82 84	21, 32, 62, 87	0
2	b	505/505 (100%)	-0.25	14 (2%) 53 58	23, 35, 71, 104	0
3	C	442/451 (98%)	-0.29	1 (0%) 95 95	23, 35, 54, 79	0
3	c	451/451 (100%)	-0.27	5 (1%) 80 83	25, 39, 60, 106	0
4	D	341/341 (100%)	-0.31	1 (0%) 94 94	20, 30, 47, 75	0
4	d	341/341 (100%)	-0.30	2 (0%) 89 91	20, 33, 59, 84	0
5	E	81/82 (98%)	0.09	3 (3%) 41 46	30, 50, 69, 81	0
5	e	82/82 (100%)	0.30	4 (4%) 29 34	39, 59, 79, 87	0
6	F	34/34 (100%)	-0.29	2 (5%) 22 26	35, 41, 64, 84	0
6	f	34/34 (100%)	-0.13	2 (5%) 22 26	40, 48, 74, 93	0
7	H	65/65 (100%)	-0.03	2 (3%) 49 54	33, 40, 57, 72	0
7	h	63/65 (96%)	0.09	2 (3%) 47 53	40, 49, 59, 66	0
8	I	35/36 (97%)	-0.22	2 (5%) 23 28	30, 36, 65, 72	0
8	i	35/36 (97%)	-0.20	2 (5%) 23 28	30, 39, 69, 76	0
9	J	36/36 (100%)	0.24	4 (11%) 5 6	34, 48, 76, 94	0
9	j	36/36 (100%)	0.32	5 (13%) 2 3	40, 53, 82, 85	0
10	K	37/37 (100%)	-0.05	0 100 100	42, 51, 67, 70	0
10	k	37/37 (100%)	0.11	1 (2%) 54 59	45, 57, 74, 85	0
11	L	37/37 (100%)	-0.36	0 100 100	22, 29, 62, 69	0
11	l	36/37 (97%)	-0.24	1 (2%) 53 58	25, 29, 68, 75	0
12	M	32/33 (96%)	-0.20	1 (3%) 49 54	26, 31, 61, 74	0
12	m	31/33 (93%)	-0.19	0 100 100	26, 32, 48, 67	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/244 (100%)	-0.05	11 (4%) 33 37	25, 41, 82, 133	0
13	o	244/244 (100%)	-0.11	12 (4%) 29 34	22, 39, 76, 127	0
14	T	29/30 (96%)	-0.59	1 (3%) 45 50	24, 31, 59, 68	0
14	t	29/30 (96%)	-0.36	2 (6%) 16 20	25, 31, 76, 94	0
15	U	97/97 (100%)	-0.24	2 (2%) 63 67	30, 41, 68, 90	0
15	u	97/97 (100%)	-0.41	2 (2%) 63 67	30, 40, 57, 83	0
16	V	137/137 (100%)	-0.47	0 100 100	25, 40, 55, 85	0
16	v	137/137 (100%)	-0.21	1 (0%) 87 89	32, 46, 65, 81	0
17	Y	27/30 (90%)	1.86	11 (40%) 0 0	53, 75, 110, 122	0
17	y	30/30 (100%)	1.03	8 (26%) 0 0	59, 71, 98, 102	0
18	X	38/38 (100%)	0.28	4 (10%) 6 7	37, 49, 76, 84	0
18	x	38/38 (100%)	0.60	3 (7%) 12 15	48, 60, 84, 103	0
19	Z	62/62 (100%)	0.87	17 (27%) 0 0	50, 65, 108, 122	0
19	z	62/62 (100%)	1.09	15 (24%) 0 0	56, 73, 115, 119	0
20	R	34/34 (100%)	1.89	15 (44%) 0 0	59, 70, 86, 92	0
20	r	31/34 (91%)	2.56	21 (67%) 0 0	69, 85, 97, 104	0
All	All	5300/5326 (99%)	-0.17	188 (3%) 44 49	20, 37, 73, 133	0

All (188) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
19	z	33	TRP	8.8
13	o	3	GLN	8.6
13	O	3	GLN	7.6
13	o	58	ASN	7.6
18	X	2	THR	7.4
1	A	13	LEU	7.3
13	O	59	LYS	7.2
17	Y	20	ALA	7.1
13	O	60	ARG	6.3
17	Y	23	THR	6.1
13	o	61	GLN	5.8
13	o	57	LYS	5.7
13	O	4	THR	5.6
19	z	35	ARG	5.6
13	o	4	THR	5.5

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Mol	Chain	Res	Type	RSRZ
9	J	8	ILE	5.4
9	J	6	GLY	5.3
20	r	26	TYR	5.2
20	R	3	TRP	5.2
17	Y	22	LEU	5.1
17	Y	21	GLN	5.1
20	R	6	LEU	5.0
13	o	56	PRO	4.8
17	Y	41	VAL	4.8
3	c	23	ALA	4.8
13	O	61	GLN	4.8
18	x	2	THR	4.7
17	y	19	ILE	4.7
18	X	3	ILE	4.7
19	z	30	PRO	4.7
20	r	3	TRP	4.7
14	t	29	ILE	4.6
20	r	9	LEU	4.6
9	j	5	GLY	4.6
20	r	6	LEU	4.5
19	Z	62	VAL	4.4
20	r	14	LEU	4.3
20	r	18	TRP	4.3
17	Y	44	GLY	4.2
13	O	62	GLU	4.1
20	r	24	LEU	4.1
6	F	12	SER	4.1
9	J	5	GLY	4.0
19	Z	7	LEU	4.0
6	F	13	TYR	3.9
13	O	56	PRO	3.9
19	z	34	ASP	3.9
19	Z	33	TRP	3.8
2	b	485	GLU	3.8
5	e	79	PHE	3.8
19	z	62	VAL	3.8
19	Z	60	PHE	3.8
13	o	5	LEU	3.7
17	Y	40	ALA	3.7
17	Y	37	PHE	3.7
1	A	11	ALA	3.6
2	b	503	THR	3.6

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Mol	Chain	Res	Type	RSRZ
3	c	24	THR	3.6
19	z	4	LEU	3.6
9	J	7	ARG	3.6
19	Z	42	LEU	3.6
19	z	41	PHE	3.5
20	R	26	TYR	3.5
17	Y	24	MET	3.5
19	z	3	ILE	3.5
2	B	505	ARG	3.5
2	b	495	PHE	3.5
19	z	60	PHE	3.5
20	R	28	VAL	3.5
3	c	146	PHE	3.4
3	c	143	TYR	3.4
2	b	127	ARG	3.4
20	r	2	ASP	3.4
19	Z	35	ARG	3.4
17	y	18	VAL	3.3
20	r	13	LEU	3.3
19	Z	4	LEU	3.3
20	r	15	ALA	3.3
6	f	12	SER	3.3
20	r	27	ALA	3.3
2	b	490	GLN	3.2
15	U	67	LEU	3.2
20	r	28	VAL	3.2
20	r	10	LEU	3.2
20	R	32	GLN	3.2
15	U	8	GLU	3.1
19	Z	38	GLN	3.1
2	b	296	ALA	3.1
17	Y	42	ARG	3.1
19	Z	3	ILE	3.1
9	j	7	ARG	3.1
1	A	12	ASN	3.1
20	R	25	PRO	3.1
17	y	17	GLU	3.1
8	i	36	ASP	3.0
2	b	502	VAL	3.0
13	o	245	PRO	3.0
7	H	66	GLY	3.0
2	b	161	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
5	E	79	PHE	2.9
17	y	40	ALA	2.9
2	b	128	THR	2.9
3	c	147	PHE	2.9
7	h	6	TRP	2.9
9	j	8	ILE	2.9
6	f	13	TYR	2.9
13	O	5	LEU	2.9
13	o	62	GLU	2.9
17	y	43	ARG	2.9
3	C	143	TYR	2.8
8	I	36	ASP	2.8
19	Z	30	PRO	2.8
2	B	502	VAL	2.8
20	R	31	VAL	2.8
2	b	506	ARG	2.8
20	R	5	VAL	2.8
15	u	53	ALA	2.8
12	M	33	GLN	2.8
1	a	11	ALA	2.7
20	r	7	VAL	2.7
19	Z	1	MET	2.7
20	r	31	VAL	2.7
20	R	29	LYS	2.7
20	r	21	ARG	2.7
20	r	23	ILE	2.7
2	b	505	ARG	2.7
5	e	13	ILE	2.7
20	R	21	ARG	2.7
13	O	57	LYS	2.6
20	r	25	PRO	2.6
2	b	489	GLU	2.6
18	x	29	ILE	2.5
18	X	39	ARG	2.5
2	b	486	LEU	2.5
9	j	6	GLY	2.5
13	o	63	ALA	2.5
8	I	34	ARG	2.5
20	R	2	ASP	2.5
10	k	17	ILE	2.5
14	t	28	ARG	2.5
20	r	4	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
20	R	27	ALA	2.5
7	h	63	LYS	2.4
19	z	36	SER	2.4
20	r	5	VAL	2.4
18	X	38	GLN	2.4
13	o	59	LYS	2.4
13	O	54	GLU	2.4
19	Z	61	VAL	2.4
19	Z	32	ASP	2.4
14	T	30	THR	2.4
19	z	31	GLN	2.4
11	l	3	PRO	2.3
20	R	13	LEU	2.3
5	e	4	THR	2.3
17	Y	43	ARG	2.3
19	z	37	LYS	2.3
2	B	295	GLY	2.3
18	x	38	GLN	2.3
13	o	60	ARG	2.2
4	D	236	ASN	2.2
7	H	6	TRP	2.2
4	d	13	GLY	2.2
5	E	17	VAL	2.2
17	y	37	PHE	2.2
2	b	494	GLY	2.2
17	y	20	ALA	2.2
2	B	127	ARG	2.1
19	Z	31	GLN	2.1
4	d	227[A]	GLU	2.1
5	E	83	LEU	2.1
20	R	18	TRP	2.1
19	Z	41	PHE	2.1
19	z	59	PHE	2.1
19	Z	45	GLY	2.1
19	z	32	ASP	2.1
5	e	84	LYS	2.1
8	i	34	ARG	2.1
19	z	14	ILE	2.1
16	v	21	LEU	2.1
20	r	29	LYS	2.1
2	B	293	ALA	2.1
15	u	9	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
20	R	14	LEU	2.1
17	y	22	LEU	2.0
19	Z	39	LEU	2.0
9	j	11	TRP	2.0
13	O	36	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
12	FME	M	1	10/11	0.95	0.14	33,47,76,79	0
14	FME	T	1	10/11	0.95	0.10	30,49,70,70	0
14	FME	t	1	10/11	0.95	0.09	26,38,64,65	0
8	FME	i	1	10/11	0.96	0.16	38,52,64,68	0
8	FME	I	1	10/11	0.96	0.13	33,53,72,72	0
12	FME	m	1	10/11	0.98	0.12	29,50,66,80	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
31	UNL	H	103	53/-	0.76	0.22	51,73,94,97	0
31	UNL	a	413	28/-	0.77	0.31	31,63,70,81	0
32	LMG	c	522	48/55	0.77	0.24	42,80,114,117	0
33	LHG	E	101	49/49	0.79	0.22	48,83,108,119	0
32	LMG	h	102	23/55	0.80	0.24	41,77,102,105	0
28	SQD	a	411	36/54	0.80	0.17	38,65,87,97	0
31	UNL	c	523	28/-	0.81	0.17	49,72,88,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
29	DGD	a	412	44/66	0.81	0.15	32,57,76,84	0
31	UNL	E	102	28/-	0.81	0.29	53,74,84,86	0
31	UNL	b	624	40/-	0.81	0.18	52,69,88,88	0
27	PL9	A	410	55/55	0.82	0.20	31,58,79,91	0
31	UNL	B	626	47/-	0.82	0.35	48,66,91,94	0
31	UNL	b	625	55/-	0.82	0.17	40,60,80,81	0
31	UNL	b	626	26/-	0.82	0.21	39,52,61,63	0
29	DGD	A	413	66/66	0.83	0.18	36,68,84,102	0
31	UNL	B	625	28/-	0.83	0.38	52,73,90,103	0
32	LMG	D	410	33/55	0.83	0.16	35,54,89,98	0
24	CLA	h	101	65/65	0.84	0.16	45,67,92,104	0
31	UNL	t	103	26/-	0.84	0.20	38,64,77,81	0
31	UNL	c	520	55/-	0.84	0.18	34,61,83,90	0
32	LMG	b	623	55/55	0.85	0.27	44,76,98,109	0
28	SQD	b	601	49/54	0.85	0.14	39,58,97,111	0
31	UNL	b	622	55/-	0.86	0.21	39,60,84,89	0
26	BCR	Y	101	40/40	0.86	0.13	37,54,73,75	0
24	CLA	c	512	65/65	0.86	0.14	42,60,99,125	0
27	PL9	a	409	55/55	0.86	0.21	36,66,86,99	0
31	UNL	X	101	55/-	0.86	0.16	33,54,76,78	0
24	CLA	C	514	65/65	0.86	0.18	45,65,91,105	0
24	CLA	C	513	65/65	0.87	0.15	33,56,93,103	0
31	UNL	M	104	53/-	0.87	0.16	36,48,88,90	0
31	UNL	C	522	47/-	0.87	0.13	44,56,66,67	0
24	CLA	B	616	60/65	0.87	0.16	23,42,93,98	0
31	UNL	J	101	28/-	0.88	0.15	50,63,71,81	0
31	UNL	M	103	26/-	0.88	0.18	39,51,59,64	0
32	LMG	K	102	48/55	0.88	0.16	48,71,92,101	0
26	BCR	h	103	40/40	0.88	0.13	31,54,78,88	0
32	LMG	c	519	37/55	0.88	0.16	41,70,83,88	0
31	UNL	T	101	47/-	0.88	0.18	38,49,65,71	0
28	SQD	f	101	41/54	0.88	0.22	55,90,116,124	0
24	CLA	c	513	65/65	0.88	0.21	40,74,109,115	0
33	LHG	e	101	42/49	0.88	0.28	58,87,114,129	0
31	UNL	m	101	28/-	0.89	0.14	38,53,74,82	0
26	BCR	H	101	40/40	0.89	0.11	30,47,67,71	0
31	UNL	x	101	55/-	0.89	0.19	39,58,75,78	0
31	UNL	B	623	28/-	0.89	0.11	35,51,67,77	0
31	UNL	I	101	41/-	0.89	0.14	40,51,76,78	0
26	BCR	k	101	40/40	0.89	0.12	41,64,77,79	0
28	SQD	A	412	39/54	0.89	0.19	41,68,96,103	0
31	UNL	C	520	28/-	0.89	0.10	33,46,50,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
28	SQD	B	622	54/54	0.89	0.13	33,60,88,102	0
31	UNL	T	102	44/-	0.89	0.19	41,57,76,77	0
31	UNL	d	412	43/-	0.89	0.20	43,58,70,77	0
31	UNL	C	521	28/-	0.90	0.11	44,54,60,67	0
24	CLA	B	601	65/65	0.90	0.14	32,65,102,107	0
32	LMG	c	524	49/55	0.90	0.13	37,54,88,107	0
24	CLA	D	404	65/65	0.90	0.15	21,42,123,126	0
24	CLA	a	407	65/65	0.90	0.15	17,36,89,116	0
24	CLA	b	617	60/65	0.90	0.14	24,44,89,98	0
32	LMG	C	501	48/55	0.91	0.15	34,57,72,109	0
32	LMG	D	407	51/55	0.91	0.17	24,58,93,98	0
26	BCR	C	515	40/40	0.91	0.13	28,39,49,64	0
31	UNL	B	620	43/-	0.91	0.11	35,49,60,70	0
32	LMG	b	621	51/55	0.91	0.12	32,51,76,91	0
28	SQD	F	101	36/54	0.91	0.15	41,74,93,99	0
26	BCR	D	405	40/40	0.91	0.12	29,46,90,104	0
31	UNL	j	101	28/-	0.91	0.12	44,56,67,68	0
24	CLA	B	615	65/65	0.91	0.12	20,38,64,87	0
31	UNL	t	102	34/-	0.91	0.13	38,51,64,77	0
26	BCR	K	101	40/40	0.91	0.12	33,56,69,76	0
24	CLA	b	616	65/65	0.91	0.13	26,41,60,72	0
24	CLA	C	507	65/65	0.92	0.12	25,42,99,113	0
24	CLA	c	507	65/65	0.92	0.15	28,45,64,65	0
24	CLA	d	405	65/65	0.92	0.13	25,49,107,114	0
32	LMG	M	101	51/55	0.92	0.11	25,47,71,81	0
29	DGD	H	102	62/66	0.92	0.12	27,48,63,78	0
26	BCR	c	521	40/40	0.92	0.15	40,56,70,75	0
26	BCR	b	619	40/40	0.93	0.09	27,41,54,56	0
32	LMG	B	621	28/55	0.93	0.12	33,50,62,66	0
26	BCR	b	620	40/40	0.93	0.10	29,50,62,66	0
28	SQD	a	410	54/54	0.93	0.13	41,68,93,95	0
24	CLA	c	508	64/65	0.93	0.12	29,48,80,108	0
26	BCR	d	406	40/40	0.93	0.12	32,56,100,106	0
24	CLA	C	508	65/65	0.93	0.13	23,40,61,67	0
24	CLA	c	502	65/65	0.93	0.13	27,42,63,71	0
29	DGD	C	516	62/66	0.93	0.12	21,40,79,95	0
29	DGD	C	517	62/66	0.93	0.11	32,56,96,109	0
24	CLA	c	504	60/65	0.93	0.12	26,46,87,91	0
31	UNL	M	102	37/-	0.93	0.11	33,47,65,67	0
32	LMG	d	411	44/55	0.93	0.13	31,55,91,97	0
24	CLA	C	506	65/65	0.93	0.17	23,39,65,76	0
29	DGD	h	104	62/66	0.93	0.11	30,51,68,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
26	BCR	b	618	40/40	0.93	0.11	25,43,56,61	0
24	CLA	c	511	65/65	0.94	0.14	43,56,76,80	0
24	CLA	A	406	65/65	0.94	0.12	21,37,99,112	0
24	CLA	a	405	65/65	0.94	0.13	22,40,97,115	0
24	CLA	C	503	65/65	0.94	0.11	27,42,60,69	0
24	CLA	b	605	65/65	0.94	0.13	18,33,82,98	0
26	BCR	A	409	40/40	0.94	0.09	21,34,44,48	0
26	BCR	B	618	40/40	0.94	0.07	22,39,51,56	0
26	BCR	B	619	40/40	0.94	0.09	21,40,62,72	0
24	CLA	b	607	65/65	0.94	0.10	22,41,77,84	0
26	BCR	C	519	40/40	0.94	0.16	29,56,68,74	0
24	CLA	b	610	65/65	0.94	0.11	26,46,64,79	0
29	DGD	c	517	62/66	0.94	0.11	31,55,92,107	0
29	DGD	c	518	62/66	0.94	0.11	26,53,78,88	0
24	CLA	b	613	65/65	0.94	0.17	20,35,45,61	0
24	CLA	b	615	65/65	0.94	0.15	24,42,81,97	0
24	CLA	B	602	65/65	0.94	0.12	22,36,63,74	0
31	UNL	B	624	46/-	0.94	0.10	39,54,66,72	0
26	BCR	b	602	40/40	0.94	0.10	23,41,66,72	0
24	CLA	B	604	65/65	0.94	0.12	18,33,77,84	0
24	CLA	B	606	65/65	0.94	0.10	24,38,76,83	0
24	CLA	c	503	65/65	0.94	0.14	24,44,55,60	0
26	BCR	c	514	40/40	0.94	0.16	35,60,72,74	0
24	CLA	C	512	65/65	0.94	0.11	34,53,69,75	0
24	CLA	c	505	65/65	0.94	0.14	24,42,66,70	0
24	CLA	c	506	65/65	0.94	0.14	25,53,110,118	0
24	CLA	B	614	65/65	0.94	0.14	16,37,88,97	0
24	CLA	A	408	54/65	0.94	0.13	16,32,62,73	0
24	CLA	c	509	65/65	0.94	0.17	29,48,64,68	0
28	SQD	A	411	52/54	0.94	0.13	33,59,89,94	0
24	CLA	c	510	65/65	0.94	0.13	32,49,73,84	0
29	DGD	C	518	62/66	0.95	0.10	26,48,79,89	0
24	CLA	b	609	65/65	0.95	0.12	25,42,58,69	0
24	CLA	C	511	65/65	0.95	0.12	28,47,67,72	0
24	CLA	A	405	65/65	0.95	0.11	15,28,41,49	0
24	CLA	b	614	65/65	0.95	0.13	15,33,74,88	0
26	BCR	c	515	40/40	0.95	0.11	25,45,64,78	0
24	CLA	d	403	65/65	0.95	0.10	16,30,44,47	0
24	CLA	C	504	65/65	0.95	0.11	22,42,54,57	0
24	CLA	C	505	59/65	0.95	0.12	26,46,75,87	0
25	PHO	a	406	64/64	0.95	0.11	22,32,41,45	0
26	BCR	t	101	40/40	0.95	0.09	25,40,56,60	0

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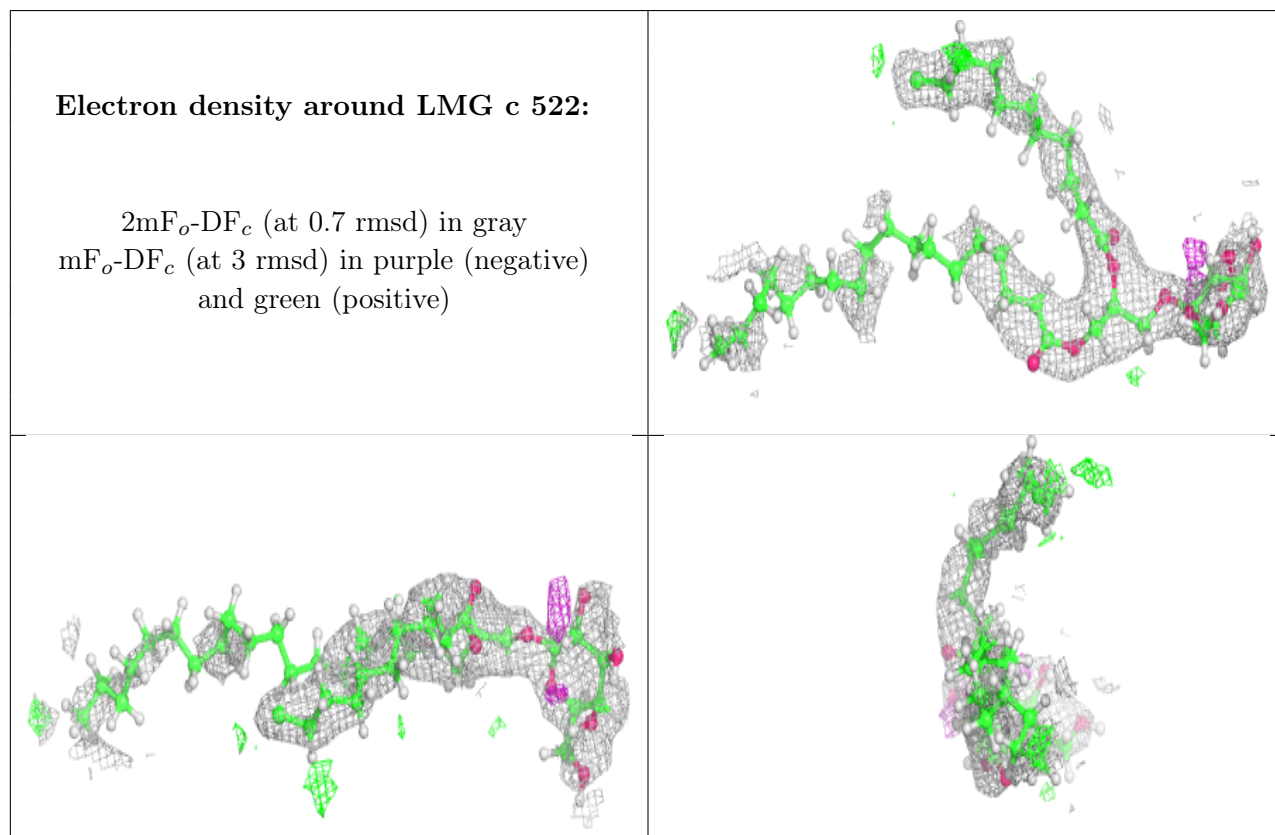
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
25	PHO	d	402	64/64	0.95	0.11	25,39,53,62	0
27	PL9	D	406	55/55	0.95	0.11	18,34,46,50	0
24	CLA	D	402	65/65	0.95	0.11	17,28,50,57	0
27	PL9	d	407	55/55	0.95	0.10	19,35,43,50	0
26	BCR	B	617	40/40	0.95	0.10	24,42,54,55	0
24	CLA	c	501	65/65	0.95	0.13	28,39,53,55	0
24	CLA	D	403	65/65	0.95	0.11	16,29,61,74	0
24	CLA	B	609	65/65	0.95	0.10	22,40,57,64	0
24	CLA	a	404	65/65	0.95	0.10	16,29,44,59	0
24	CLA	B	613	65/65	0.95	0.12	17,30,65,73	0
24	CLA	C	502	65/65	0.95	0.11	22,36,50,60	0
24	CLA	b	603	65/65	0.95	0.14	24,44,69,80	0
24	CLA	C	509	65/65	0.95	0.12	24,42,96,114	0
33	LHG	D	411	49/49	0.95	0.11	26,44,69,81	0
26	BCR	a	408	40/40	0.95	0.09	17,32,48,53	0
33	LHG	d	408	49/49	0.95	0.11	31,51,85,94	0
33	LHG	d	410	39/49	0.95	0.10	32,48,71,76	0
24	CLA	C	510	65/65	0.95	0.14	22,46,61,72	0
24	CLA	B	610	65/65	0.96	0.15	18,32,43,48	0
24	CLA	d	404	65/65	0.96	0.11	19,33,63,70	0
24	CLA	B	612	65/65	0.96	0.15	17,32,49,59	0
24	CLA	b	606	65/65	0.96	0.12	20,35,50,52	0
25	PHO	A	407	64/64	0.96	0.10	16,28,39,44	0
25	PHO	D	401	64/64	0.96	0.09	21,33,48,50	0
24	CLA	B	603	65/65	0.96	0.13	17,34,66,68	0
24	CLA	b	608	65/65	0.96	0.11	16,36,69,79	0
33	LHG	D	408	49/49	0.96	0.12	19,42,59,63	0
33	LHG	D	409	47/49	0.96	0.10	20,45,83,99	0
24	CLA	B	607	65/65	0.96	0.10	15,34,62,70	0
24	CLA	B	605	65/65	0.96	0.14	15,30,44,61	0
24	CLA	b	611	65/65	0.96	0.14	19,38,53,61	0
33	LHG	d	409	49/49	0.96	0.12	22,39,62,67	0
24	CLA	b	612	65/65	0.96	0.10	19,32,48,58	0
29	DGD	c	516	62/66	0.96	0.11	22,41,77,90	0
33	LHG	l	101	49/49	0.96	0.10	28,46,61,67	0
34	HEM	F	102	43/43	0.96	0.12	35,49,65,69	0
24	CLA	b	604	65/65	0.97	0.11	21,35,67,77	0
24	CLA	B	608	65/65	0.97	0.10	17,34,59,63	0
24	CLA	B	611	65/65	0.97	0.12	18,32,46,54	0
33	LHG	L	101	49/49	0.97	0.11	25,41,56,66	0
23	BCT	d	401	4/4	0.97	0.20	29,29,38,46	0
34	HEM	e	102	43/43	0.97	0.11	43,55,79,79	0

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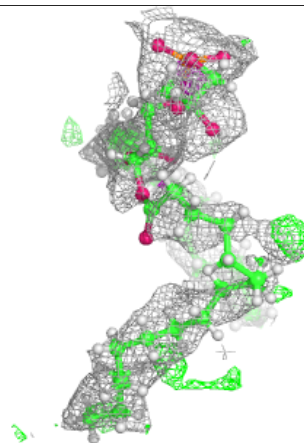
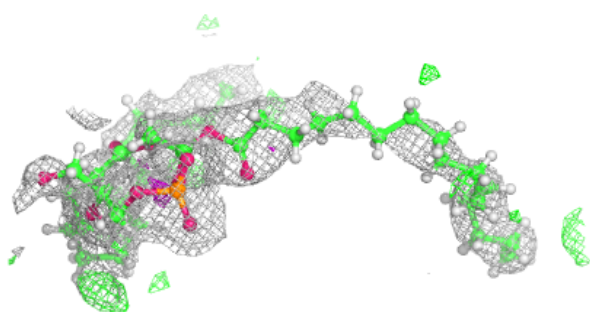
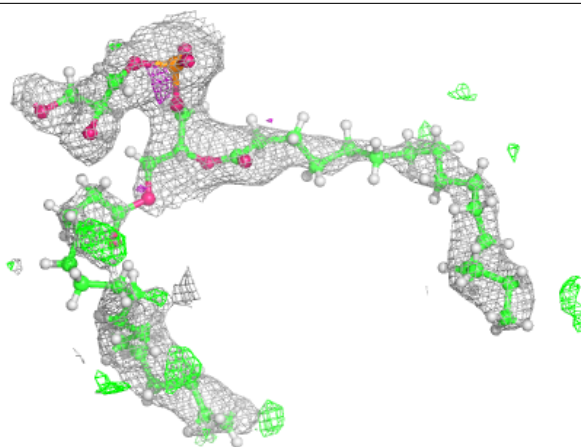
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
35	HEC	v	201	43/43	0.97	0.13	27,36,47,54	0
35	HEC	V	201	43/43	0.98	0.11	22,33,42,48	0
21	FE2	a	401	1/1	0.99	0.06	33,33,33,33	0
22	CL	A	402	1/1	0.99	0.07	25,25,25,25	0
22	CL	a	402	1/1	0.99	0.06	28,28,28,28	0
22	CL	a	403	1/1	0.99	0.03	25,25,25,25	0
30	OEX	A	414	10/10	0.99	0.11	19,29,33,33	0
30	OEX	a	414	10/10	0.99	0.11	23,29,33,34	1
23	BCT	A	404	4/4	0.99	0.13	28,28,30,36	0
21	FE2	A	401	1/1	0.99	0.08	28,28,28,28	0
22	CL	A	403	1/1	1.00	0.06	29,29,29,29	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

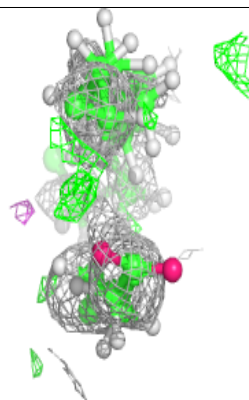
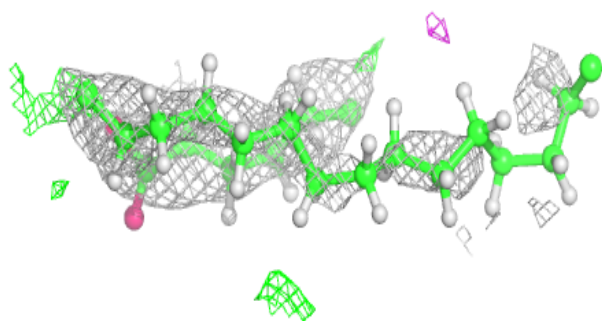
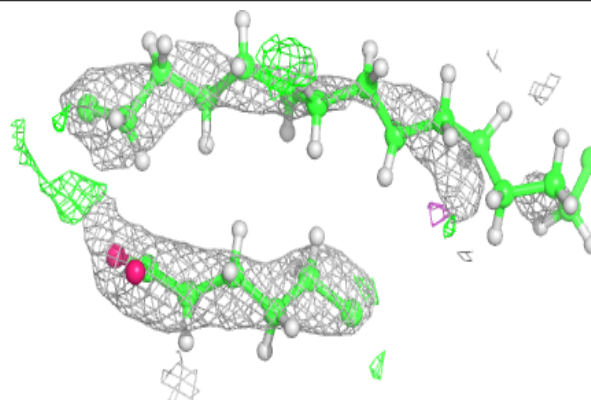


Electron density around LHG E 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

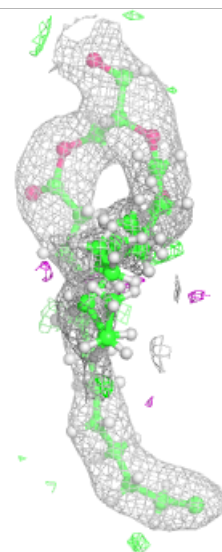
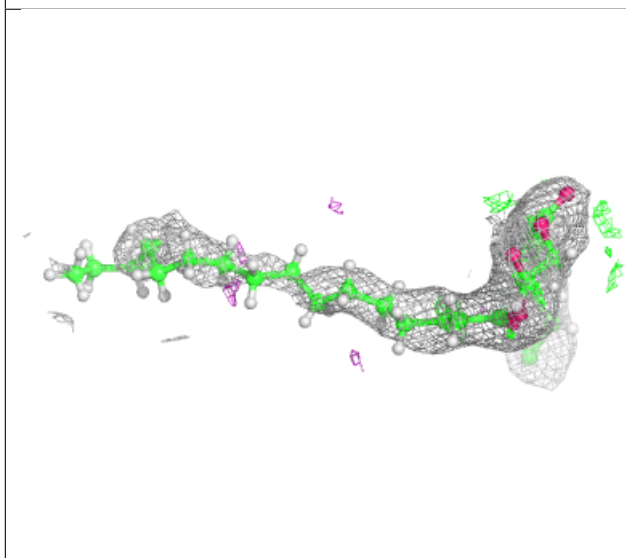
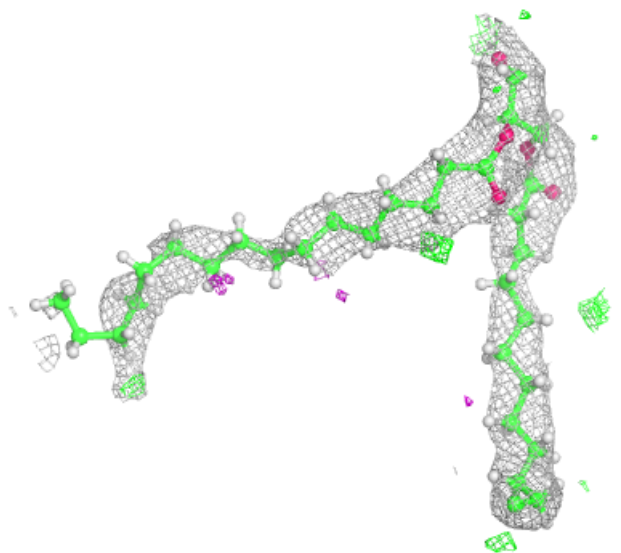
**Electron density around LMG h 102:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



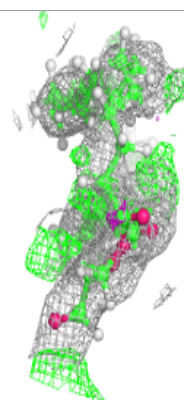
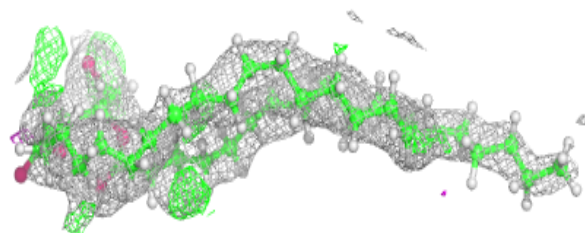
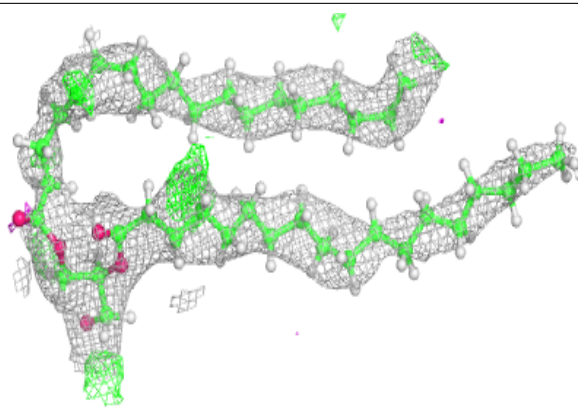
Electron density around SQD a 411:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

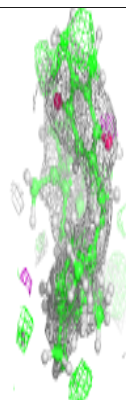
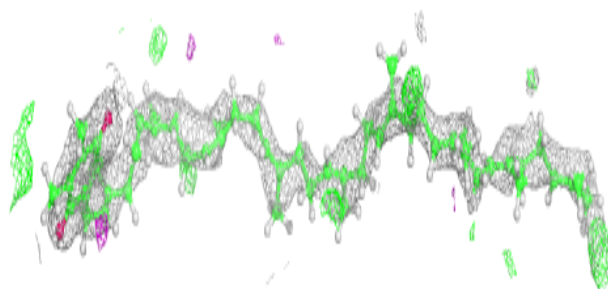
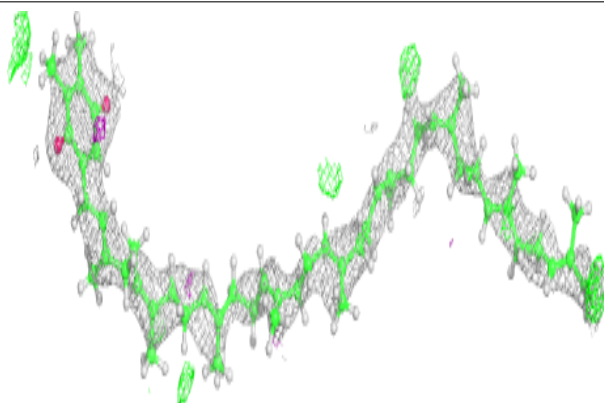


Electron density around DGD a 412:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

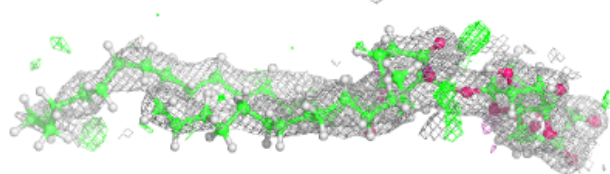
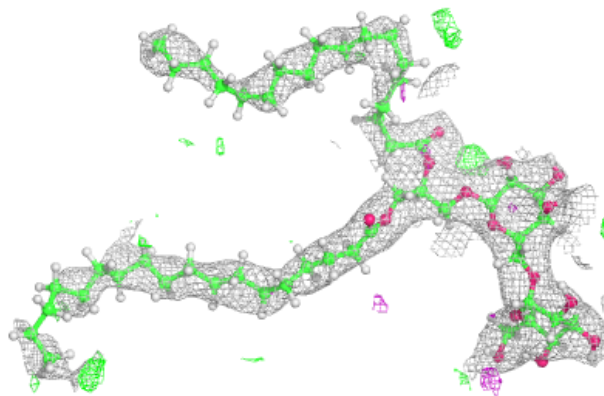
**Electron density around PL9 A 410:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

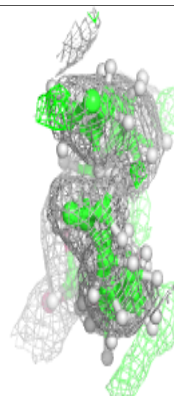
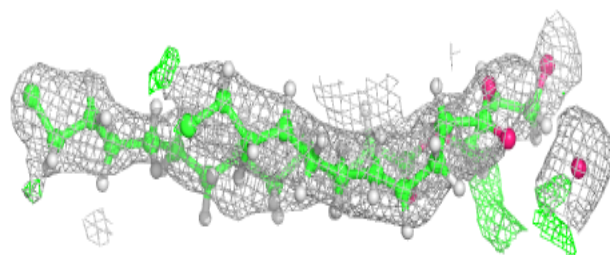
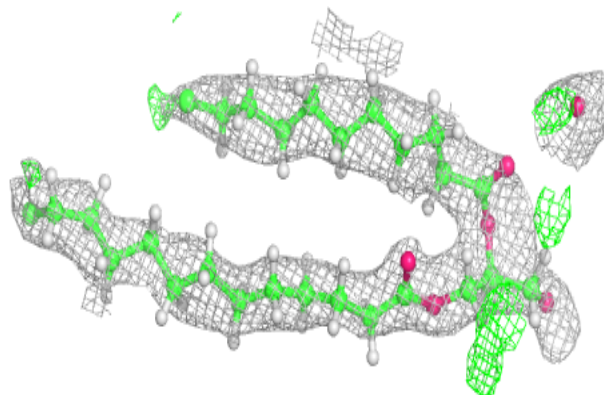


Electron density around DGD A 413:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

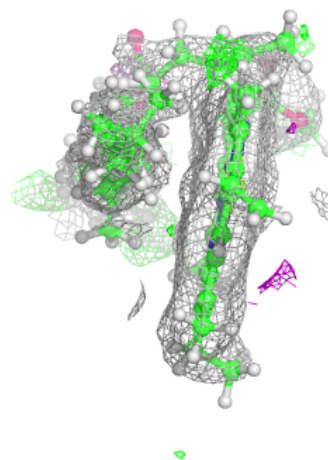
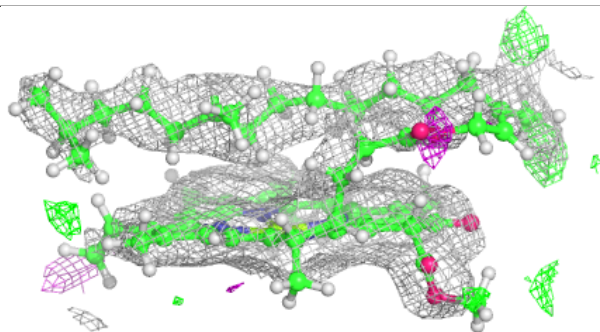
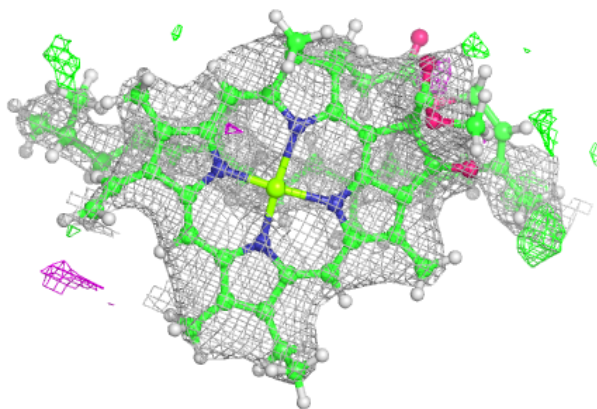
**Electron density around LMG D 410:**

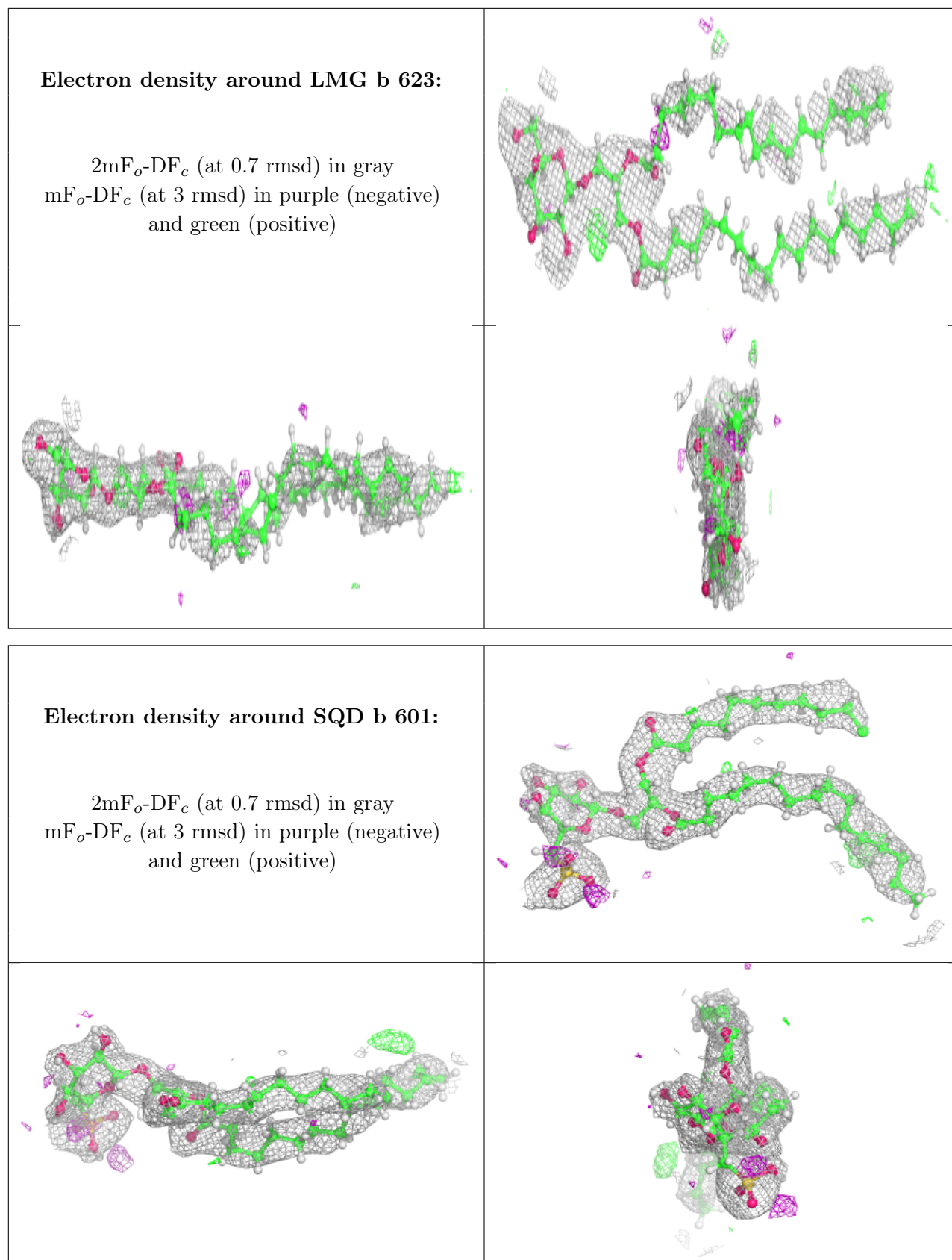
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

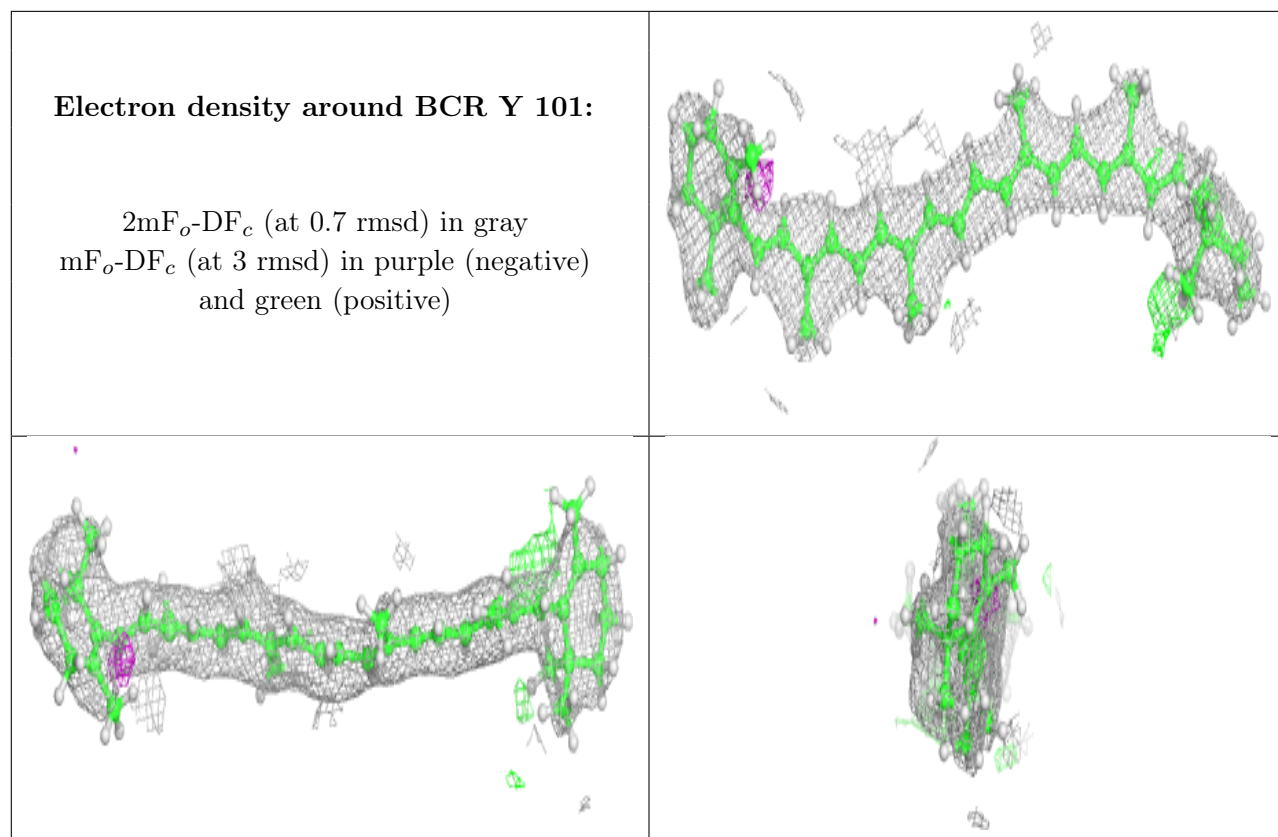


Electron density around CLA h 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

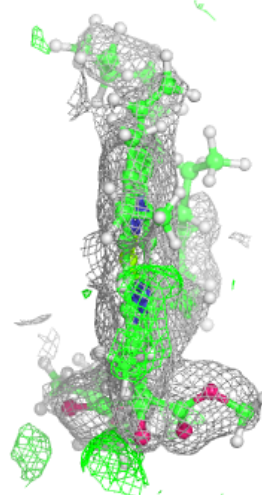
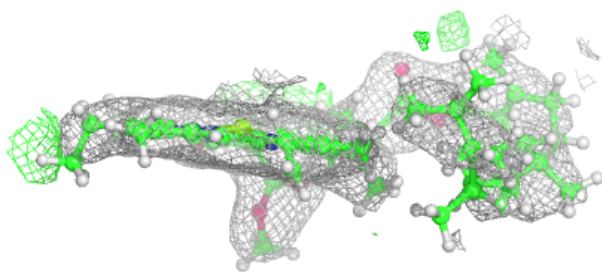
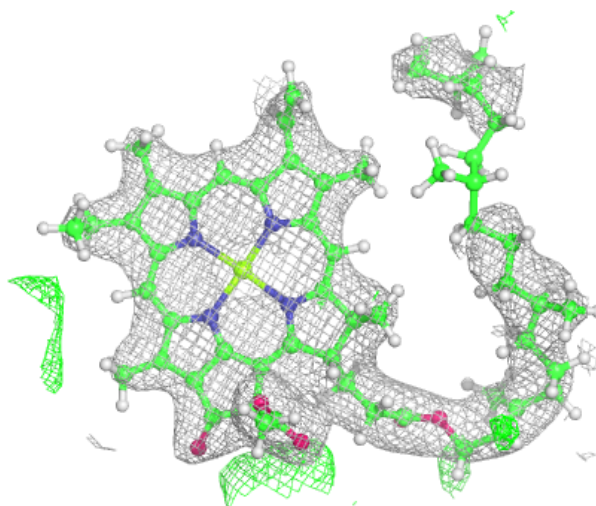






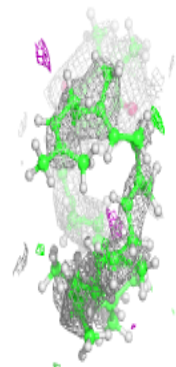
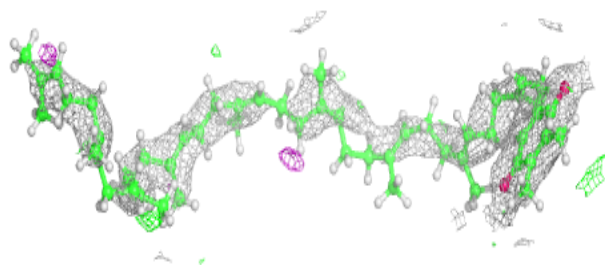
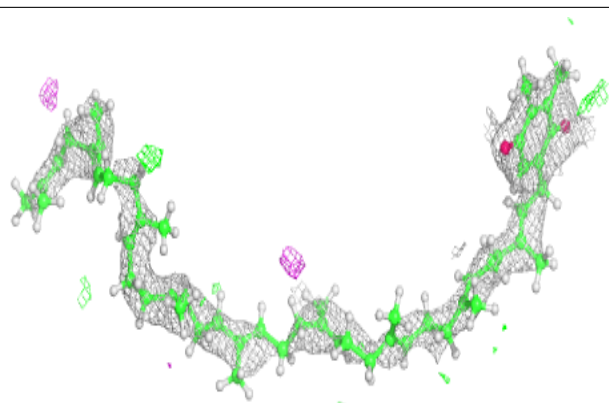
Electron density around CLA c 512:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

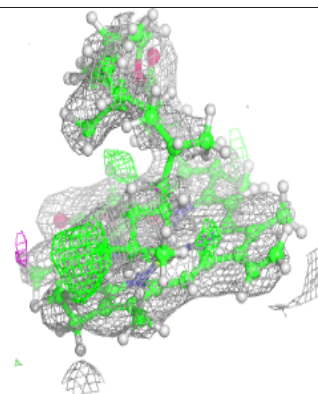
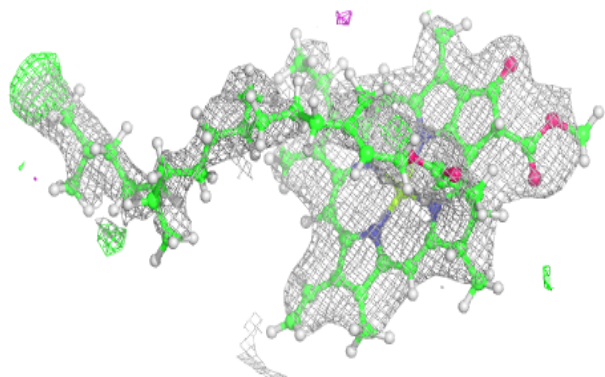
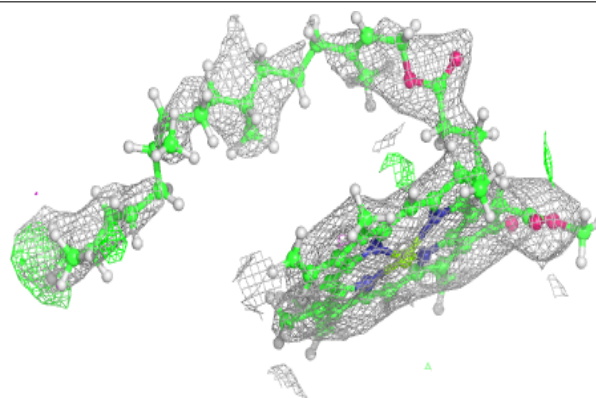


Electron density around PL9 a 409:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

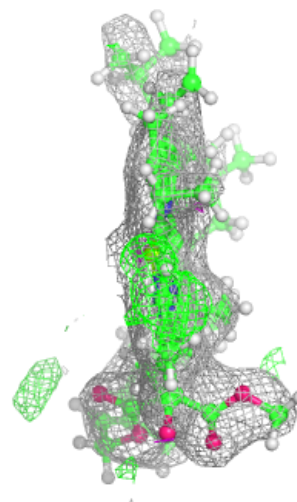
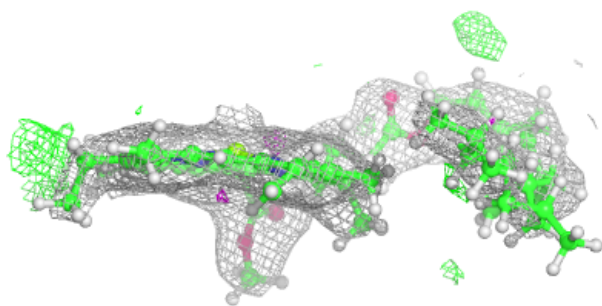
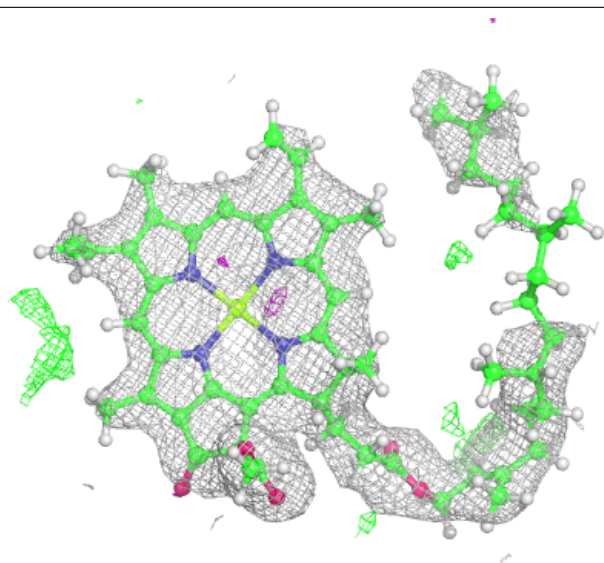
**Electron density around CLA C 514:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



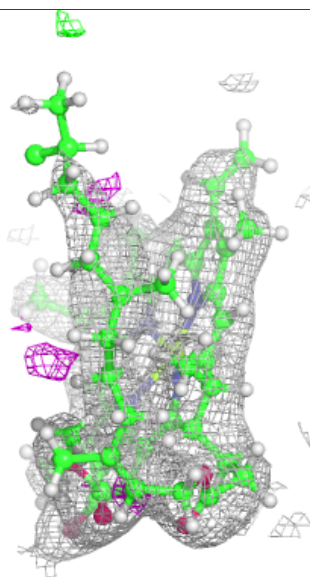
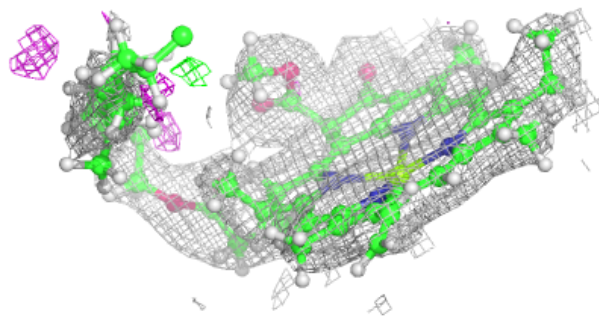
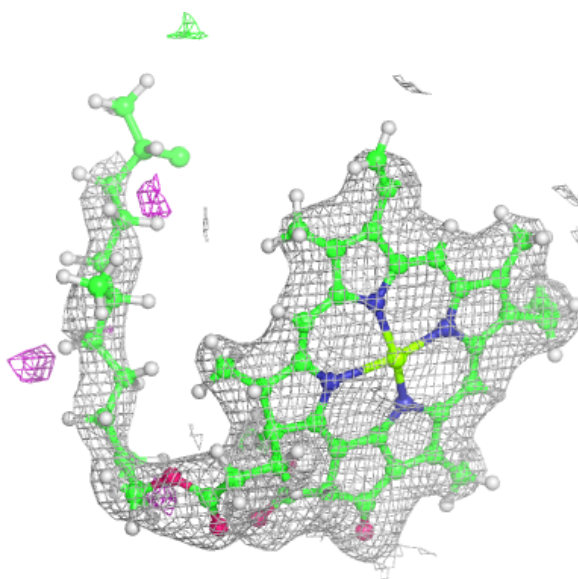
Electron density around CLA C 513:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



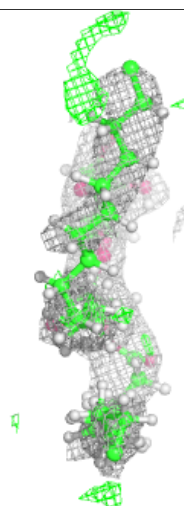
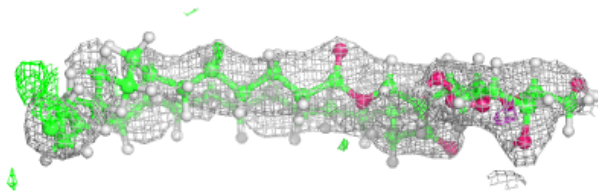
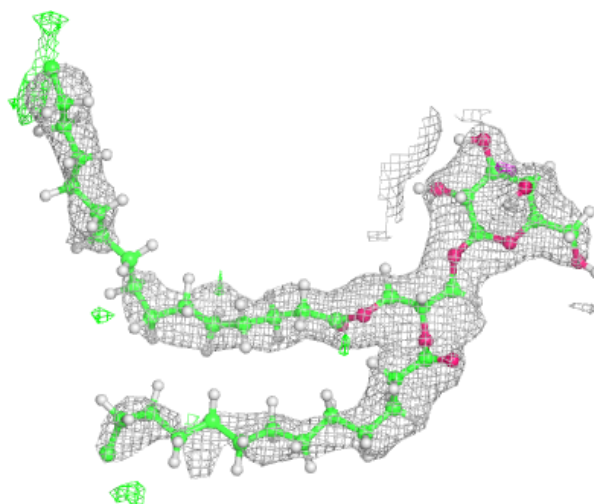
Electron density around CLA B 616:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



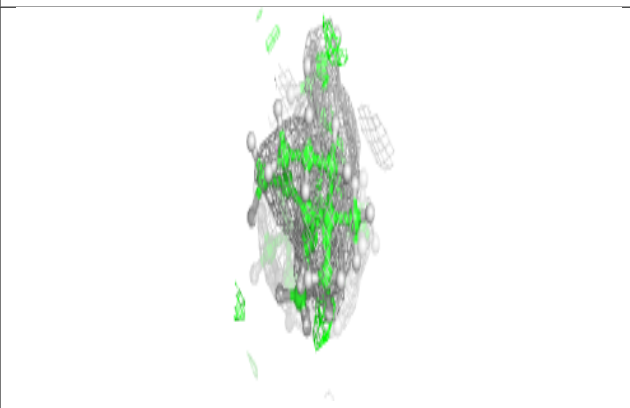
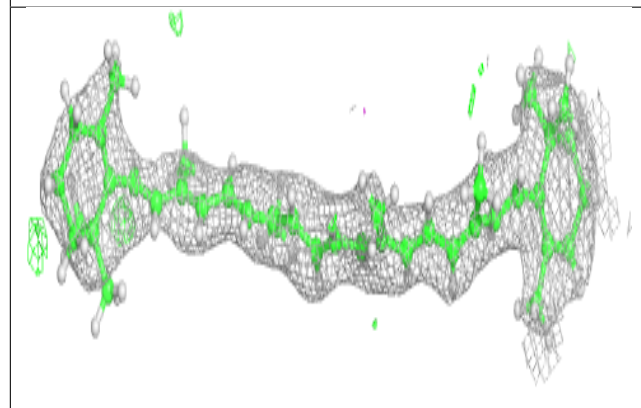
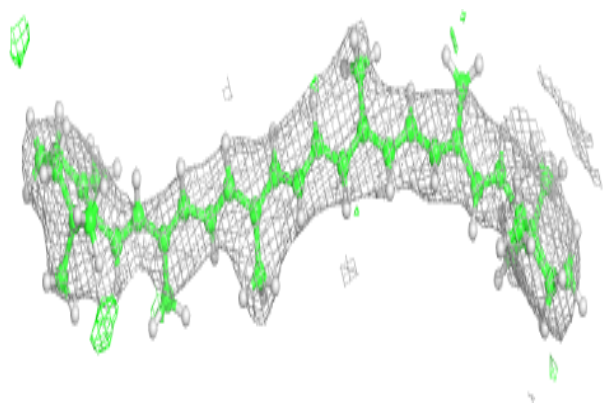
Electron density around LMG K 102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

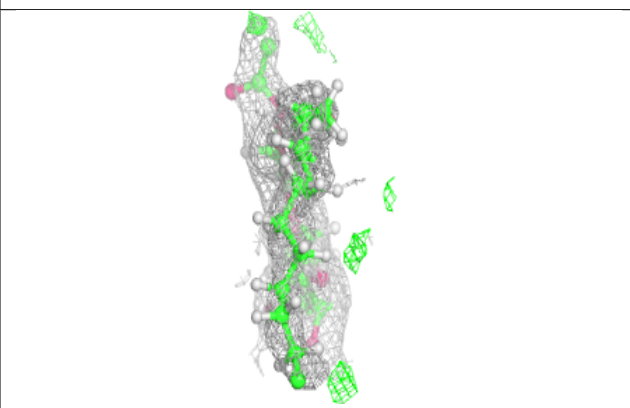
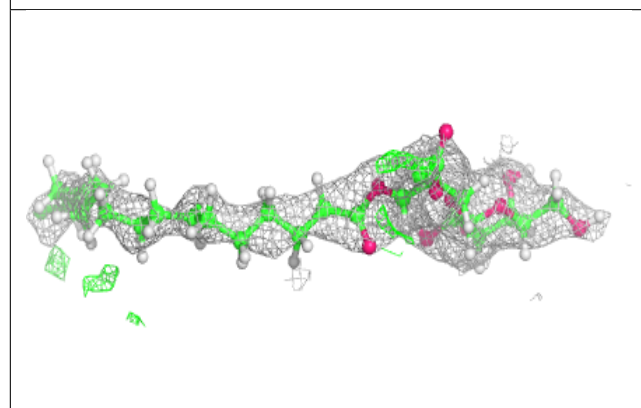
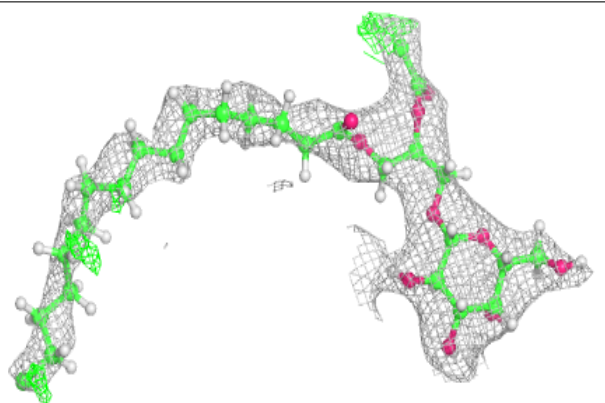


Electron density around BCR h 103:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

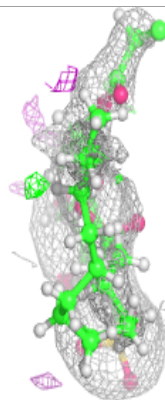
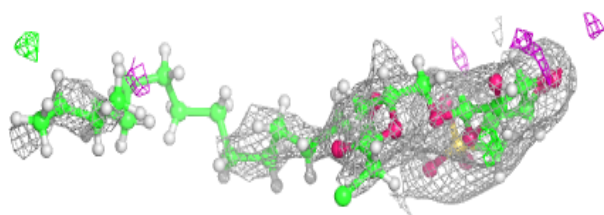
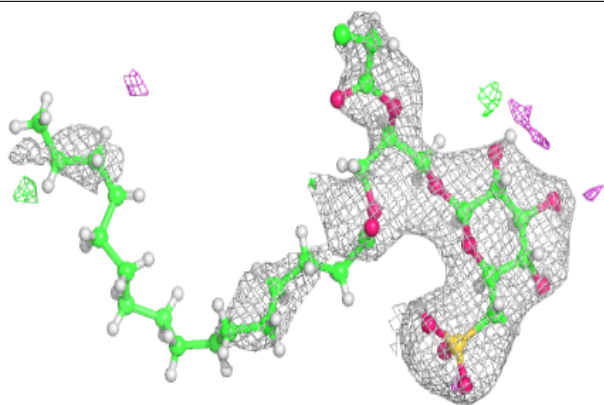
**Electron density around LMG c 519:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

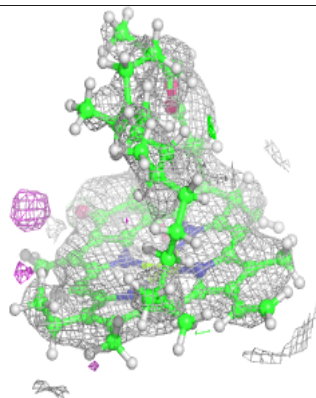
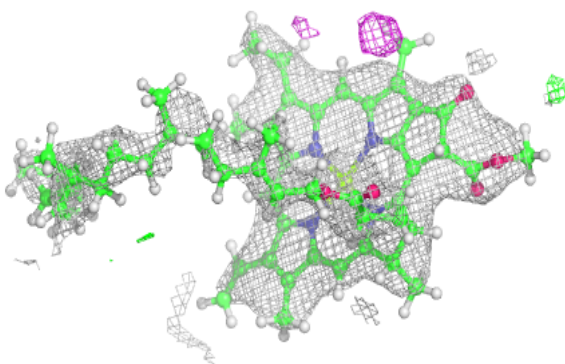
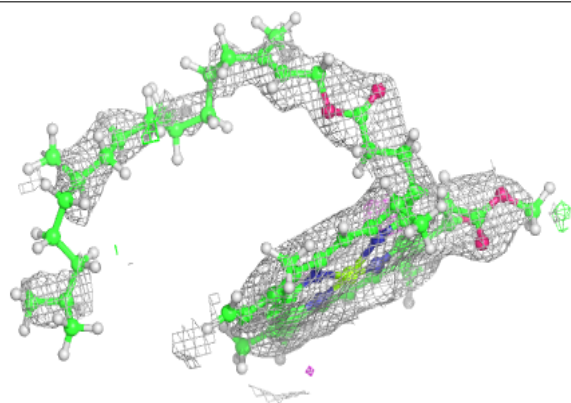


Electron density around SQD f 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

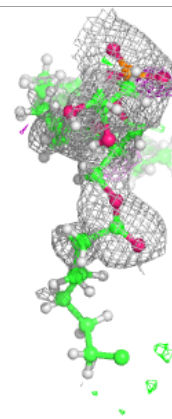
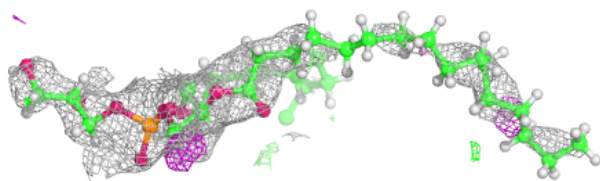
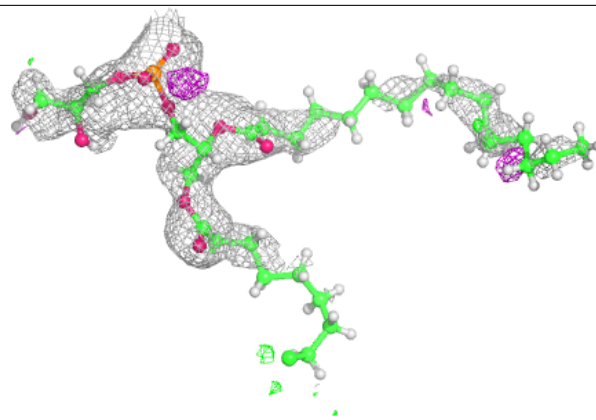
**Electron density around CLA c 513:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

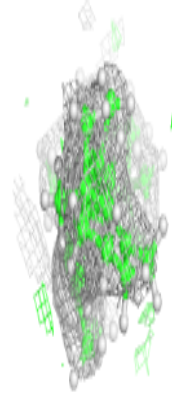
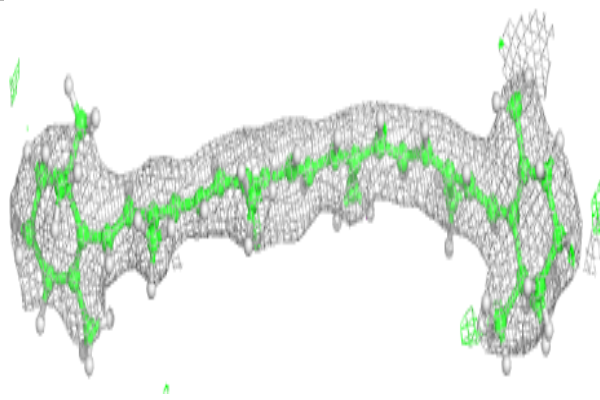
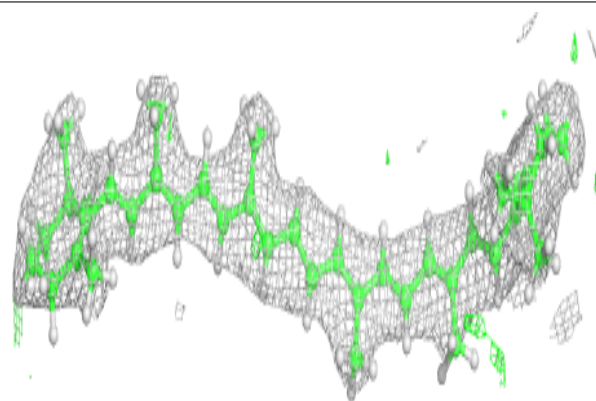


Electron density around LHG e 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

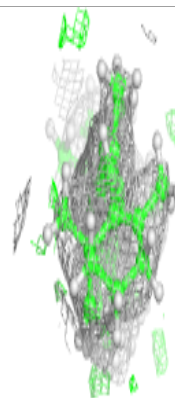
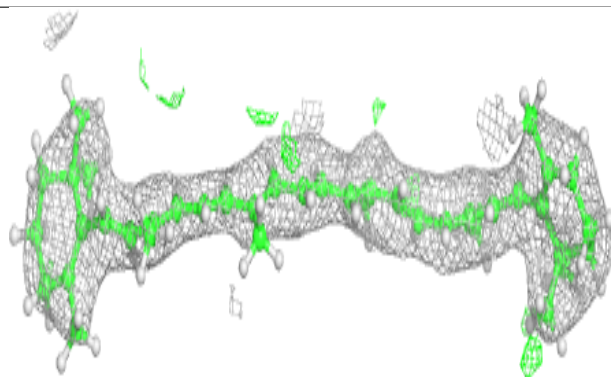
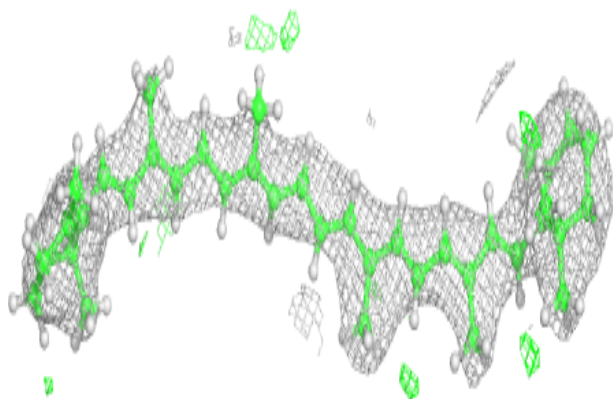
**Electron density around BCR H 101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



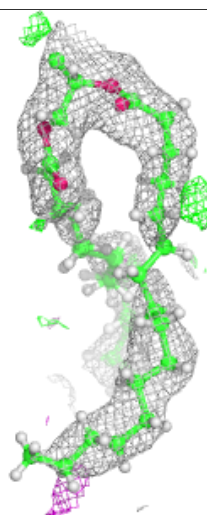
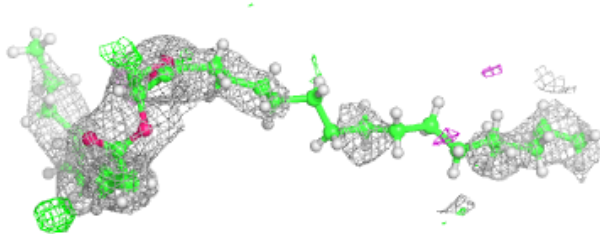
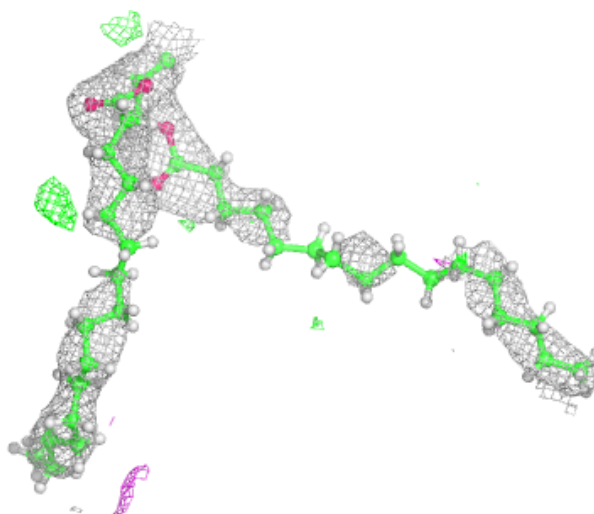
Electron density around BCR k 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



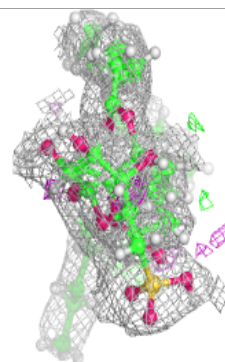
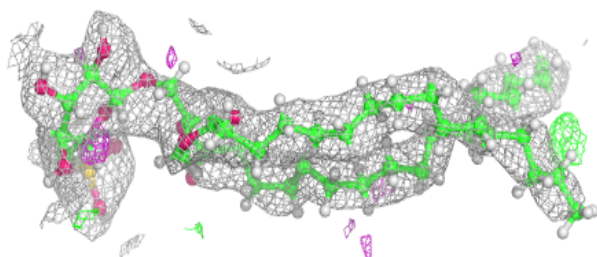
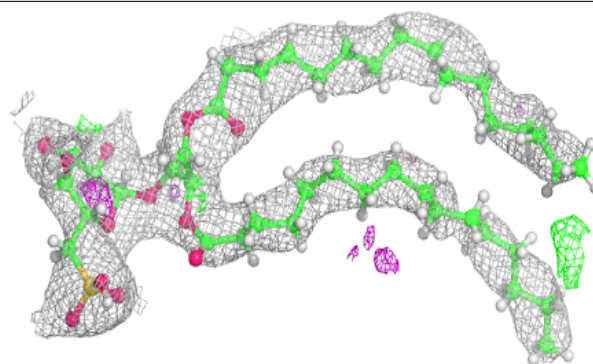
Electron density around SQD A 412:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

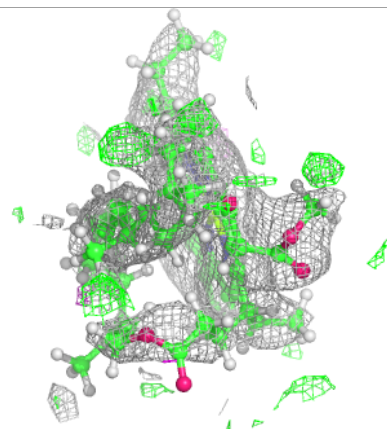
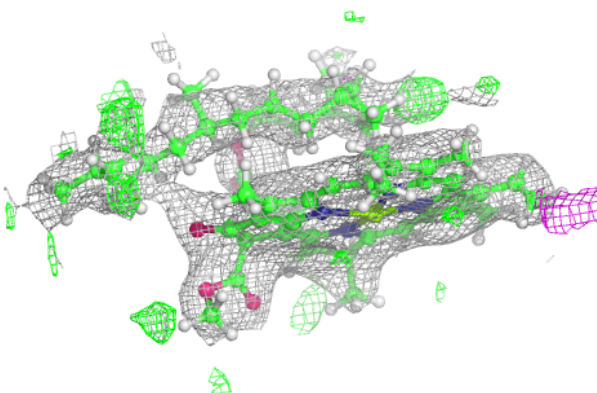
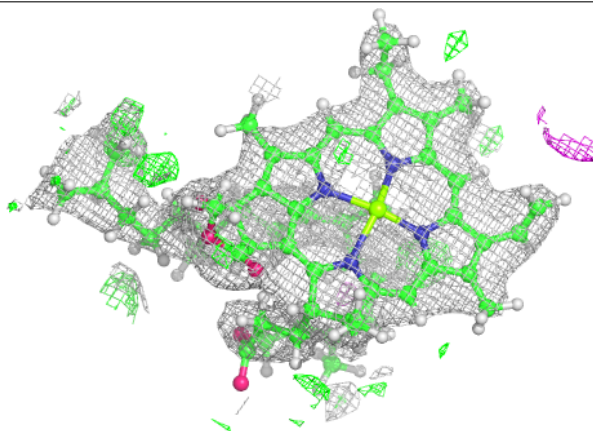


Electron density around SQD B 622:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

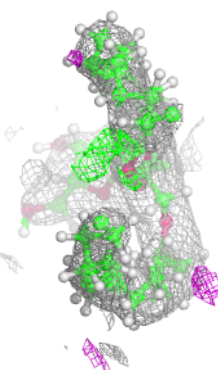
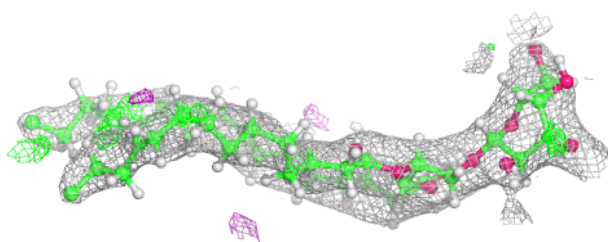
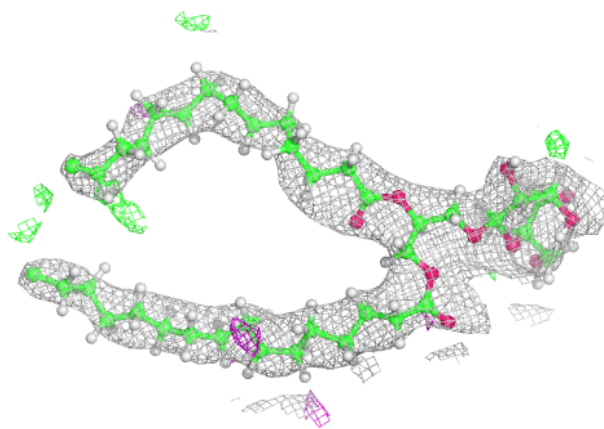
**Electron density around CLA B 601:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

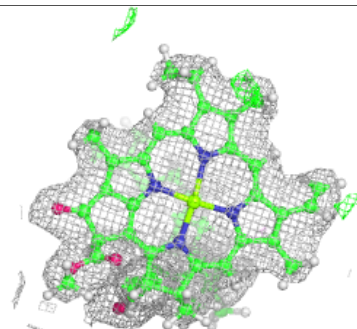
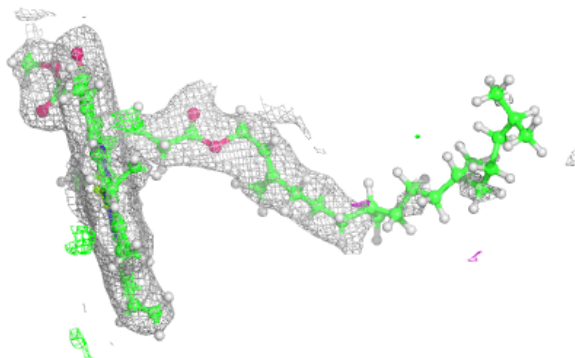
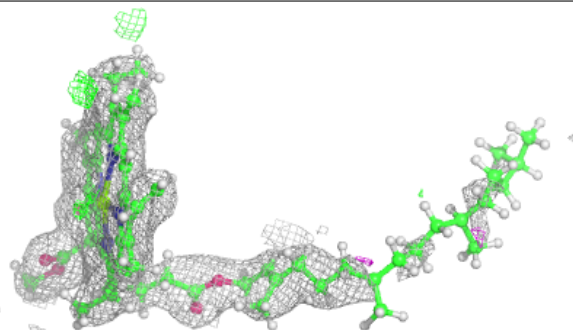


Electron density around LMG c 524:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

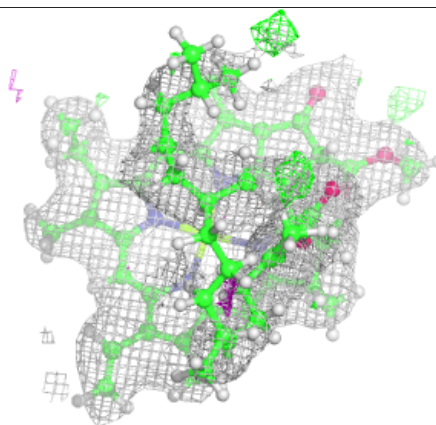
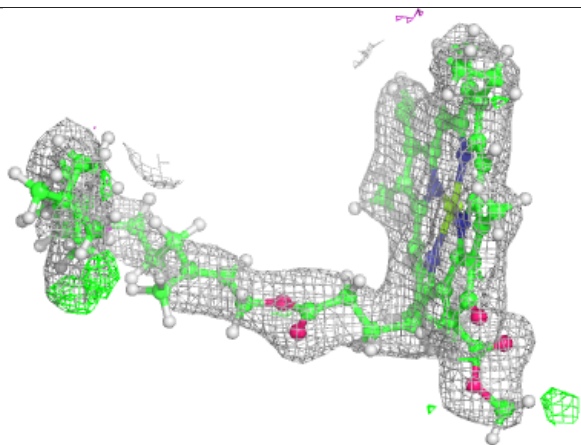
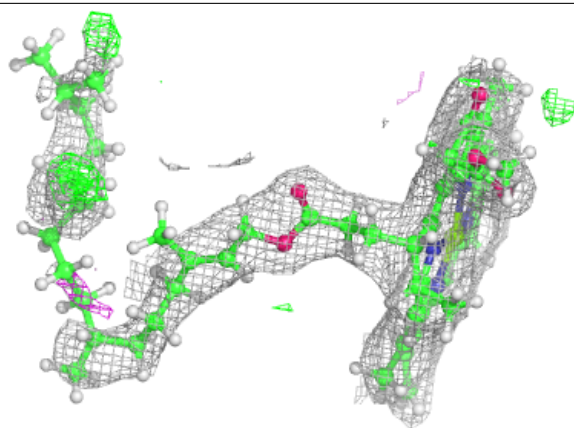
**Electron density around CLA D 404:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



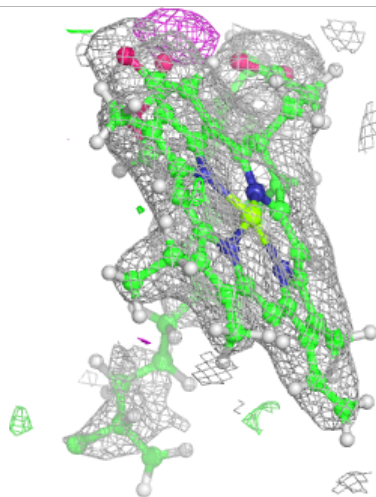
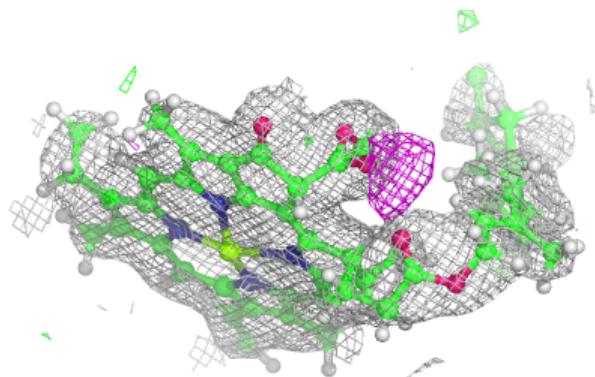
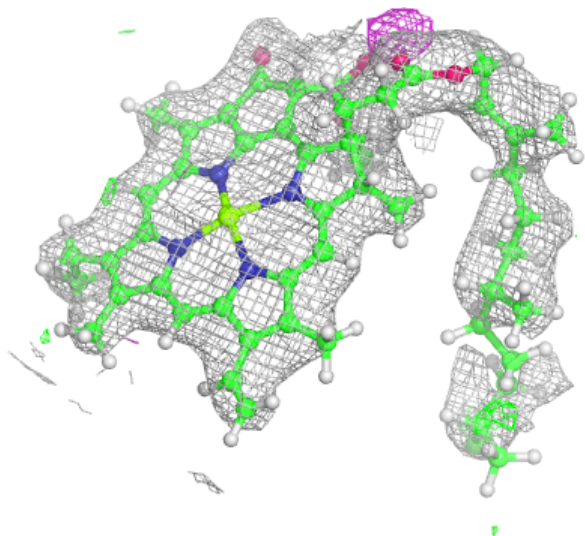
Electron density around CLA a 407:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



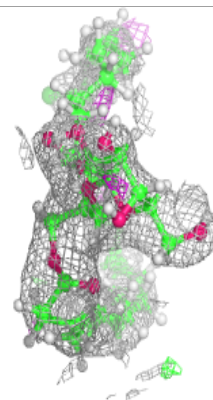
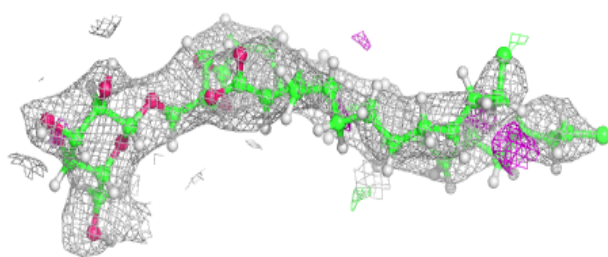
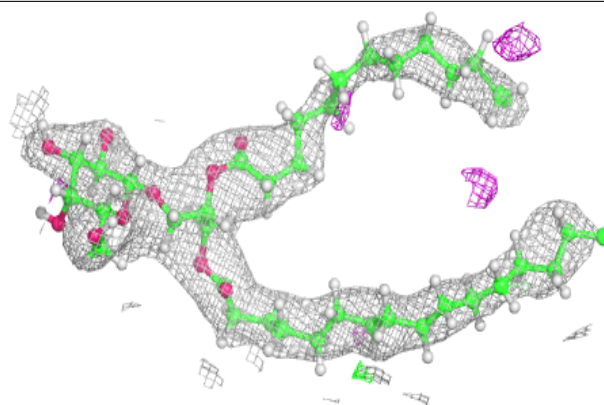
Electron density around CLA b 617:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

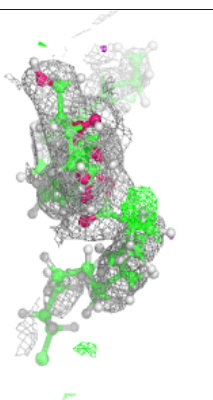
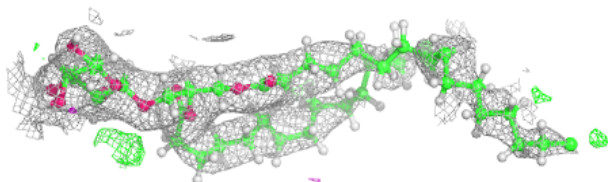
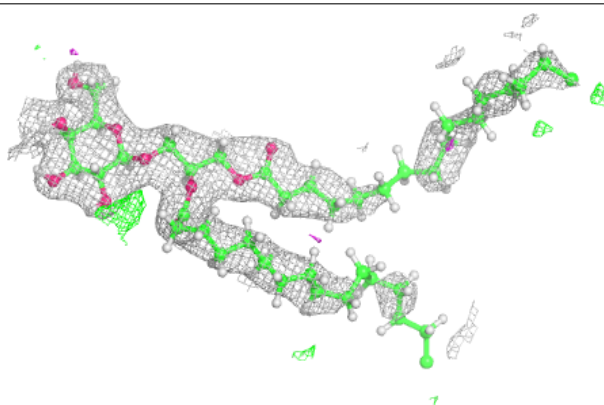


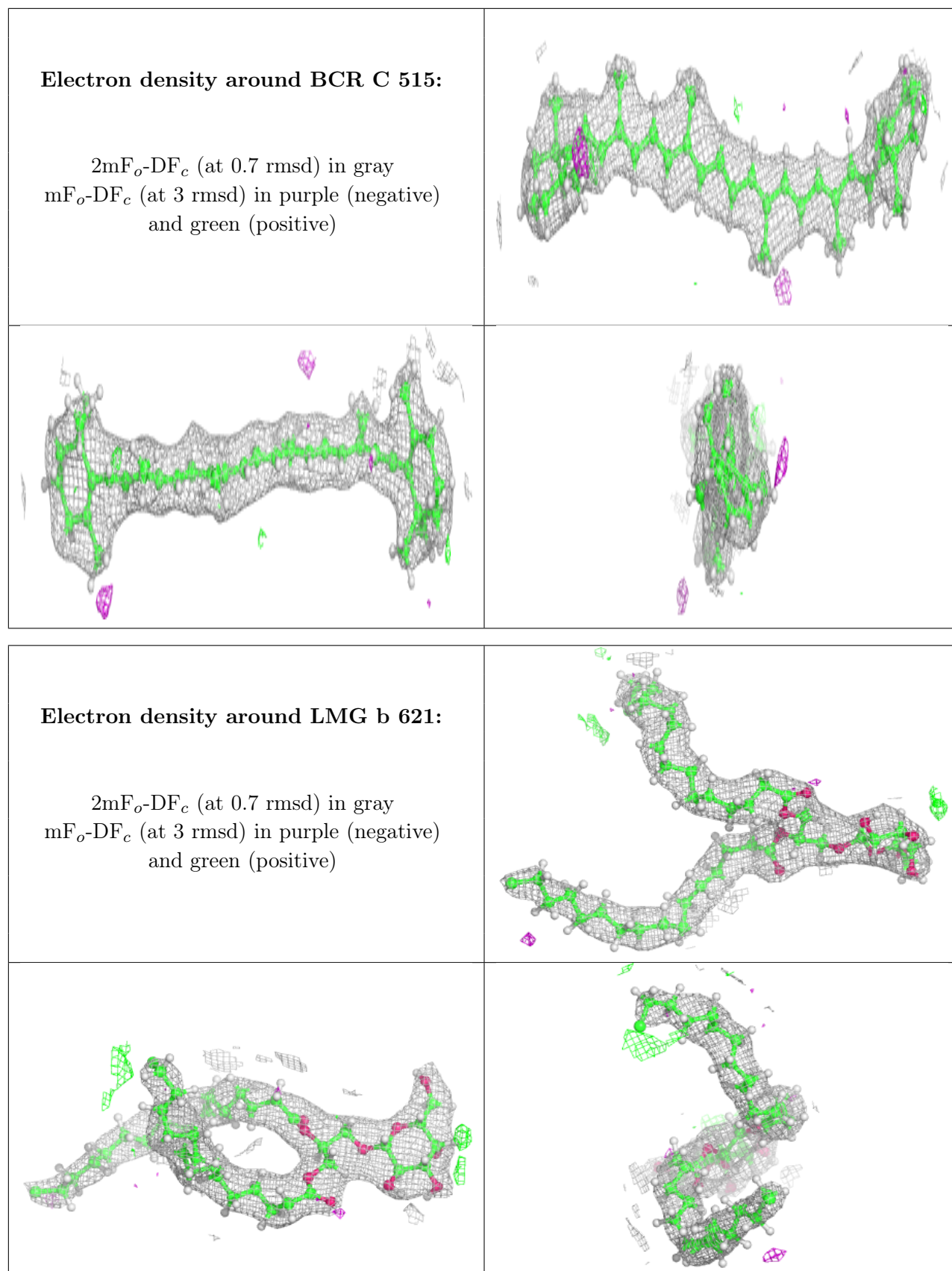
Electron density around LMG C 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around LMG D 407:**

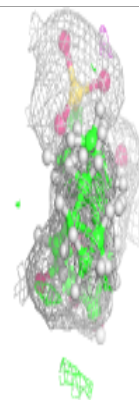
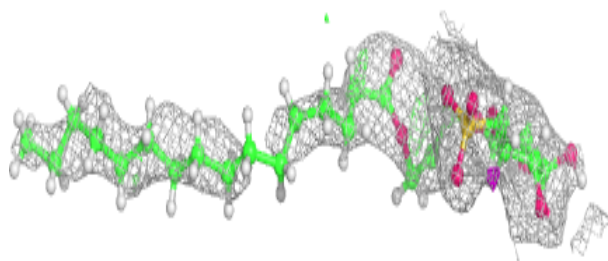
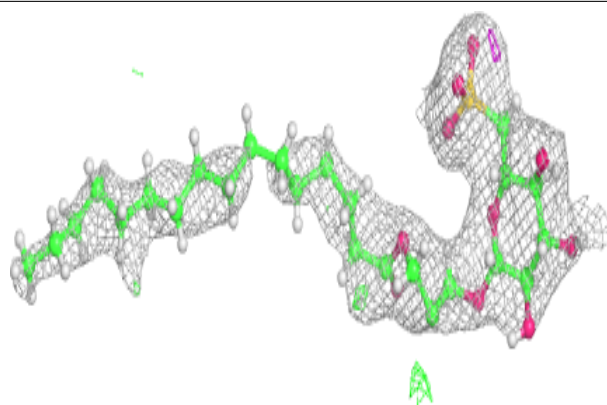
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



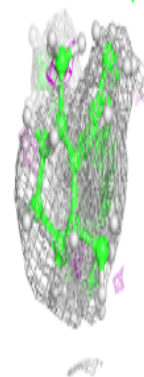
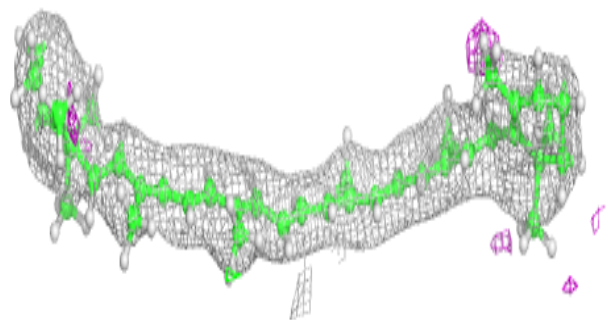
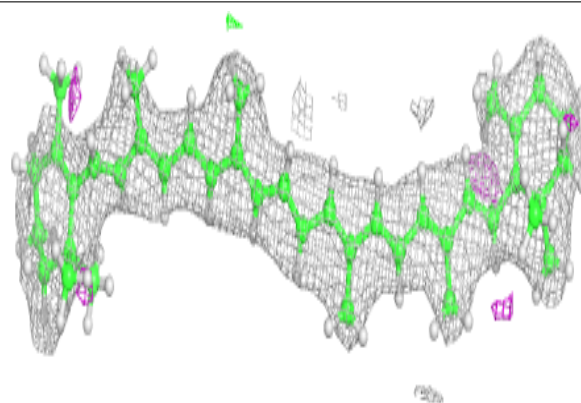


Electron density around SQD F 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

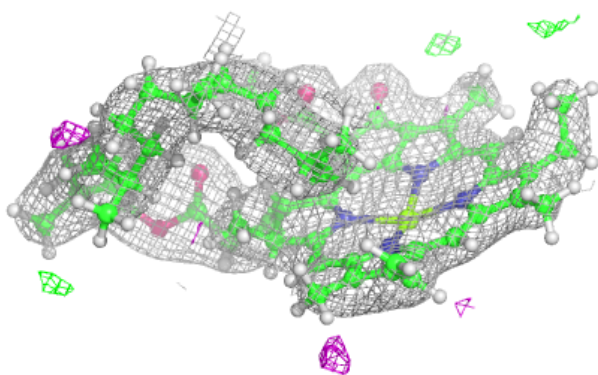
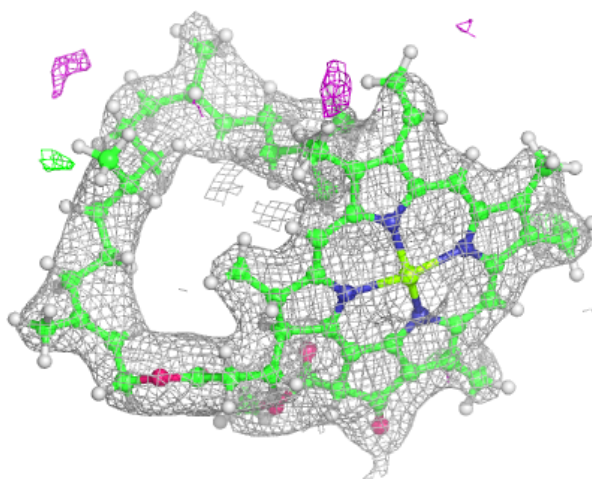
**Electron density around BCR D 405:**

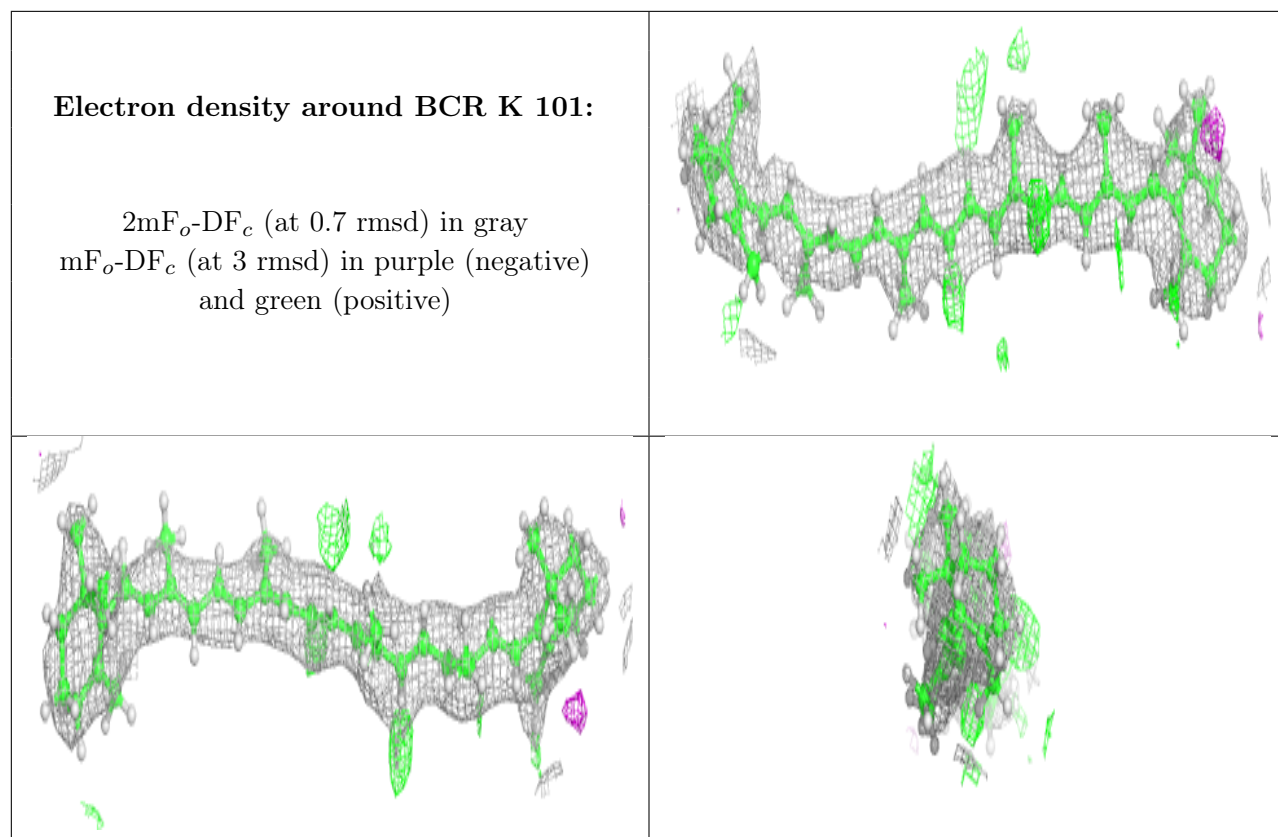
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA B 615:

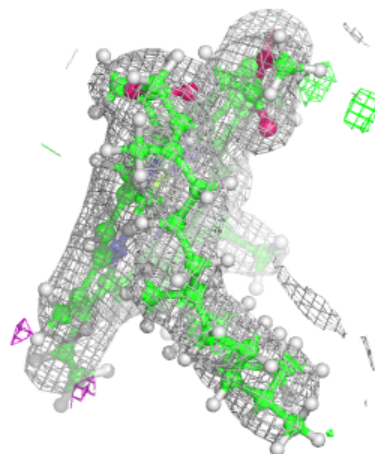
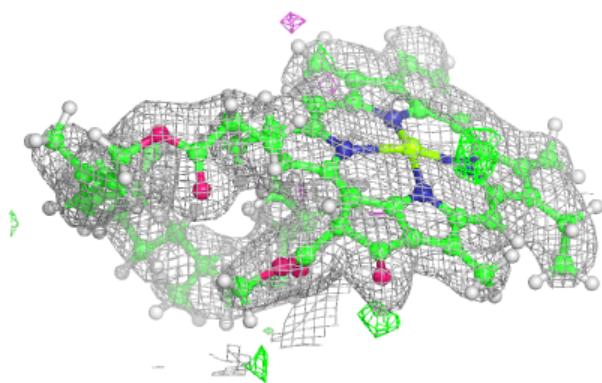
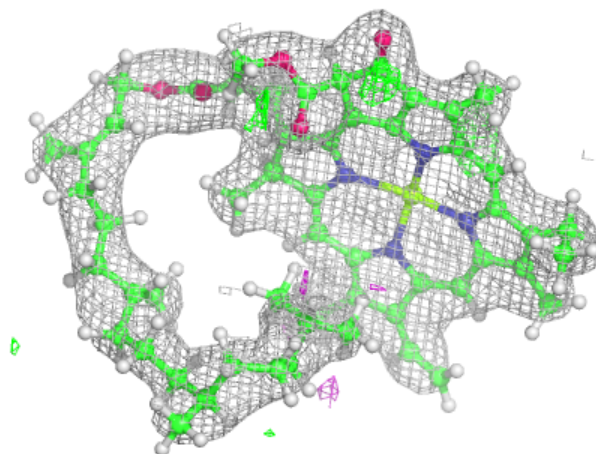
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





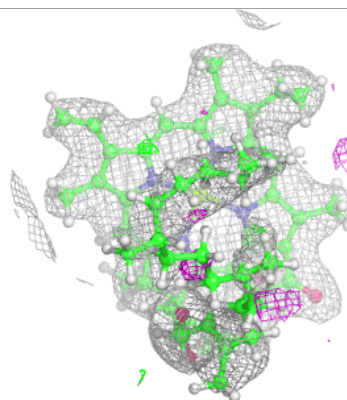
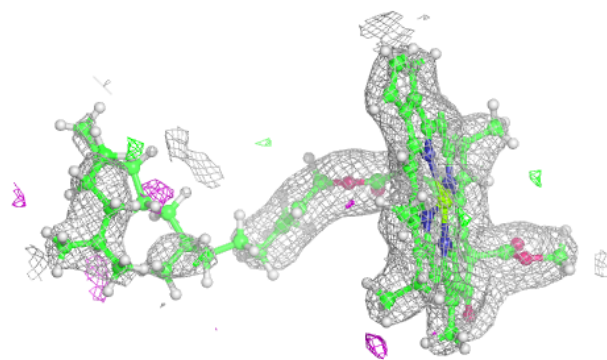
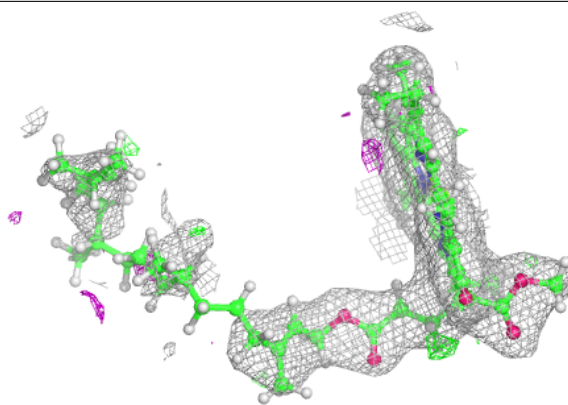
Electron density around CLA b 616:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



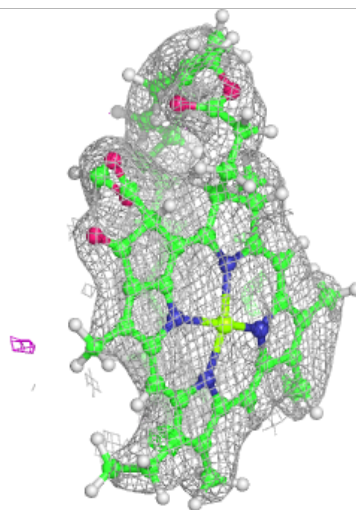
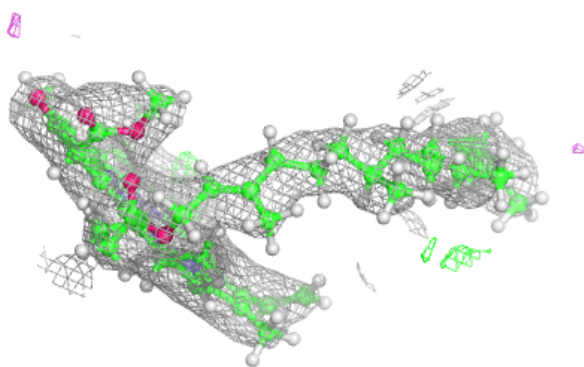
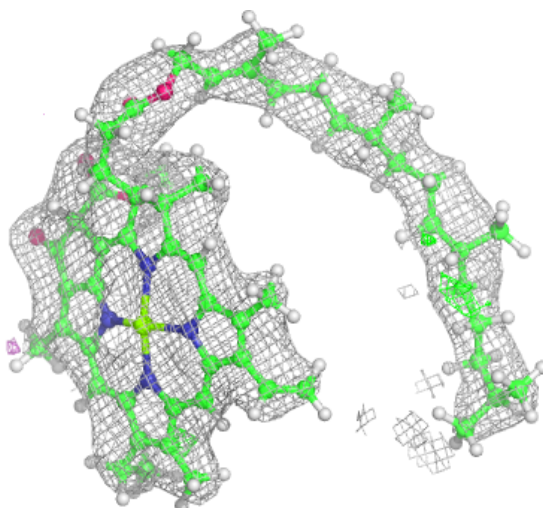
Electron density around CLA C 507:

$2mF_o-DF_c$ (at 0.7 rnsd) in gray
 mF_o-DF_c (at 3 rnsd) in purple (negative)
and green (positive)



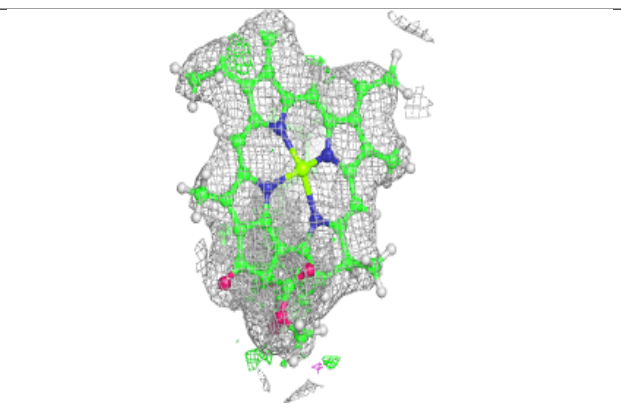
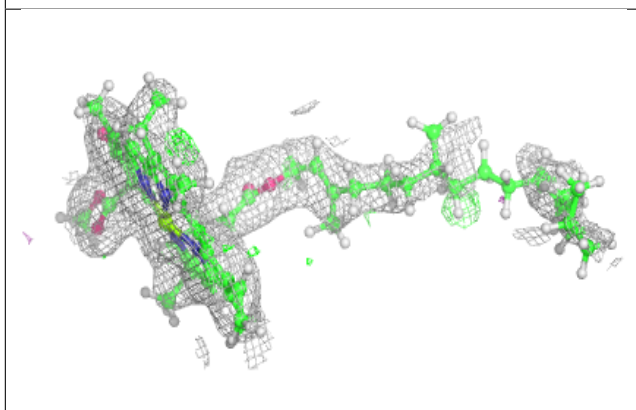
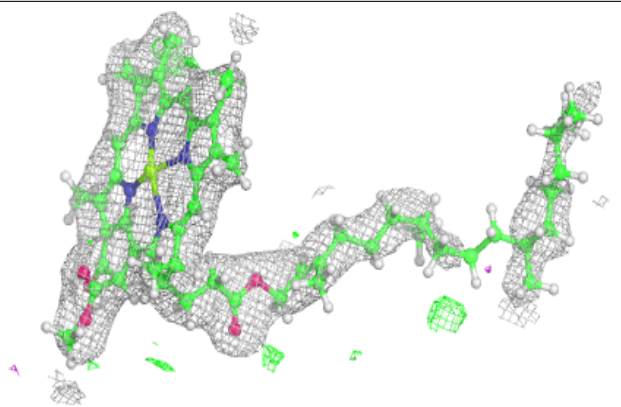
Electron density around CLA c 507:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

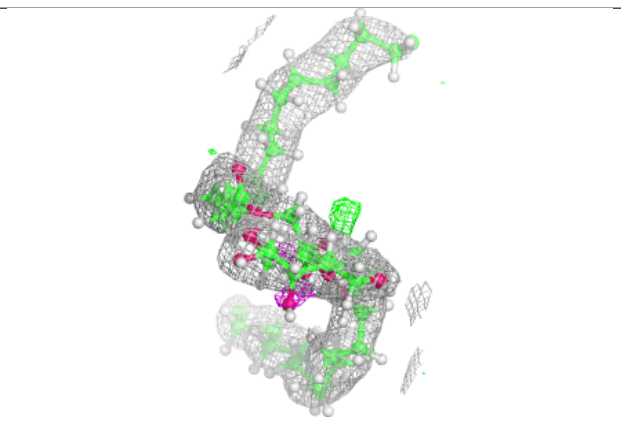
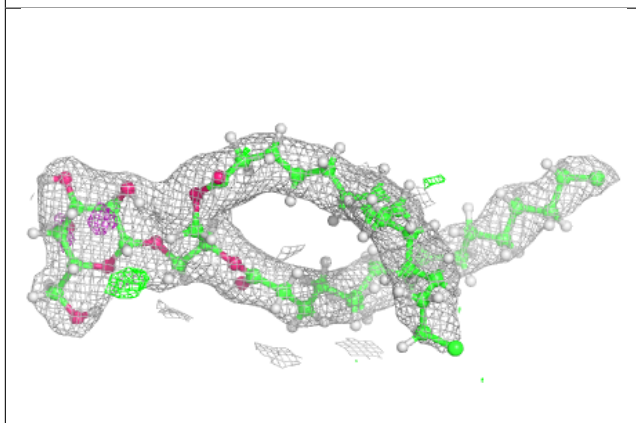
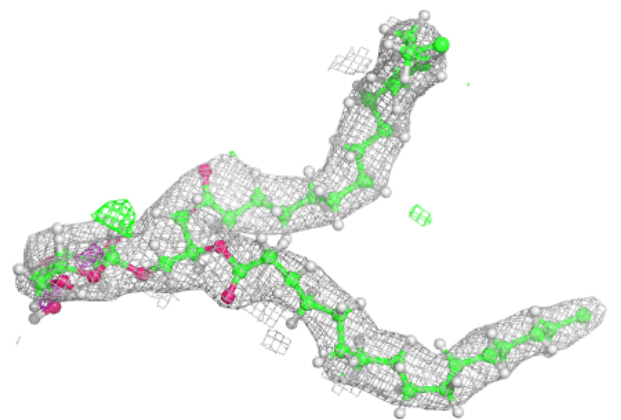


Electron density around CLA d 405:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

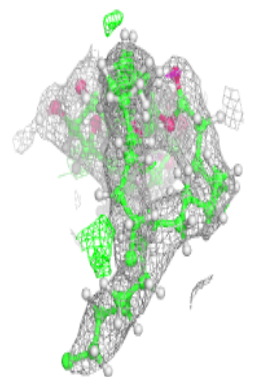
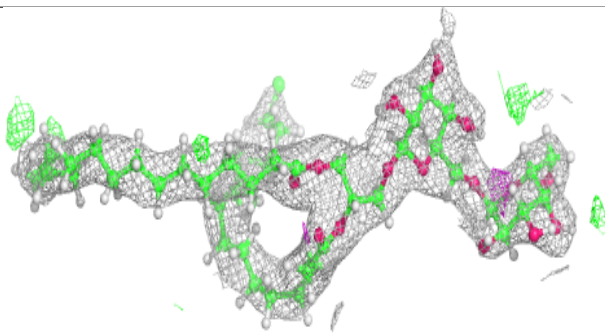
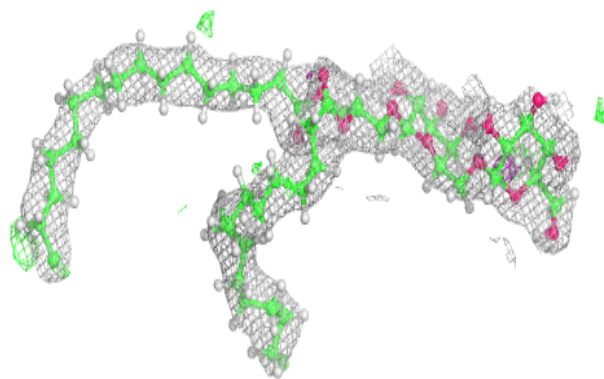
**Electron density around LMG M 101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

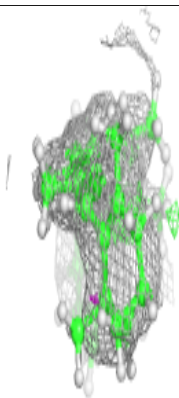
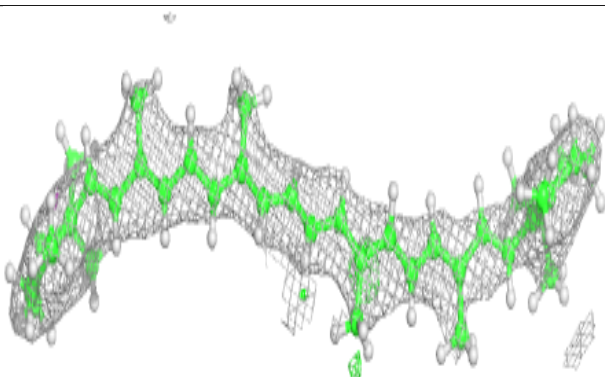
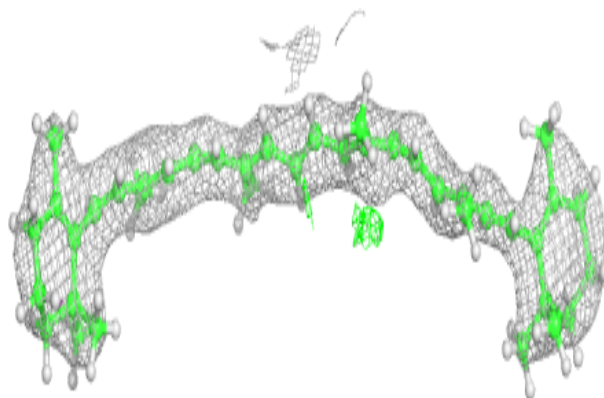


Electron density around DGD H 102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

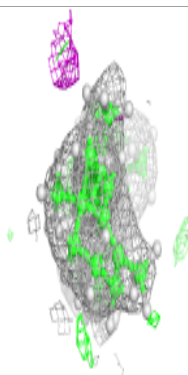
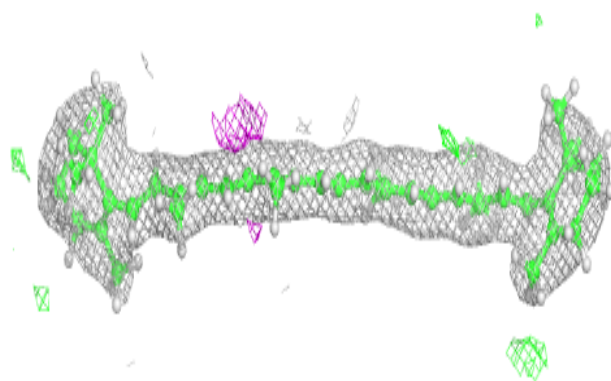
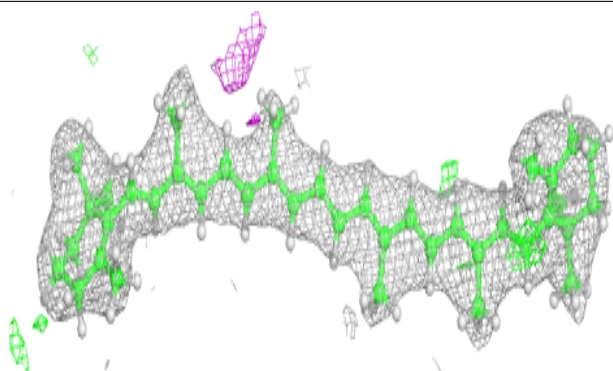
**Electron density around BCR c 521:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

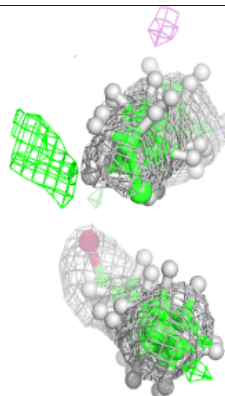
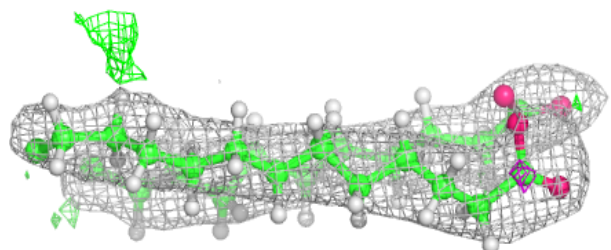
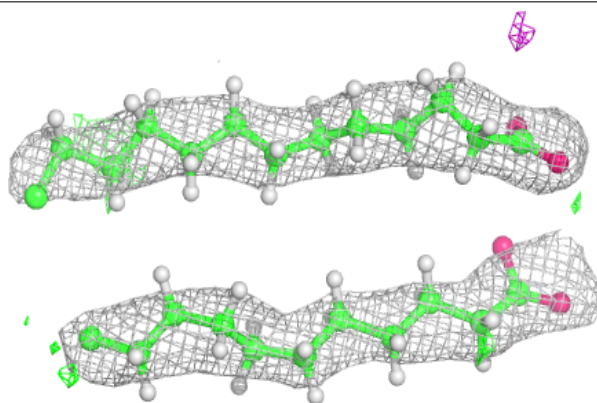


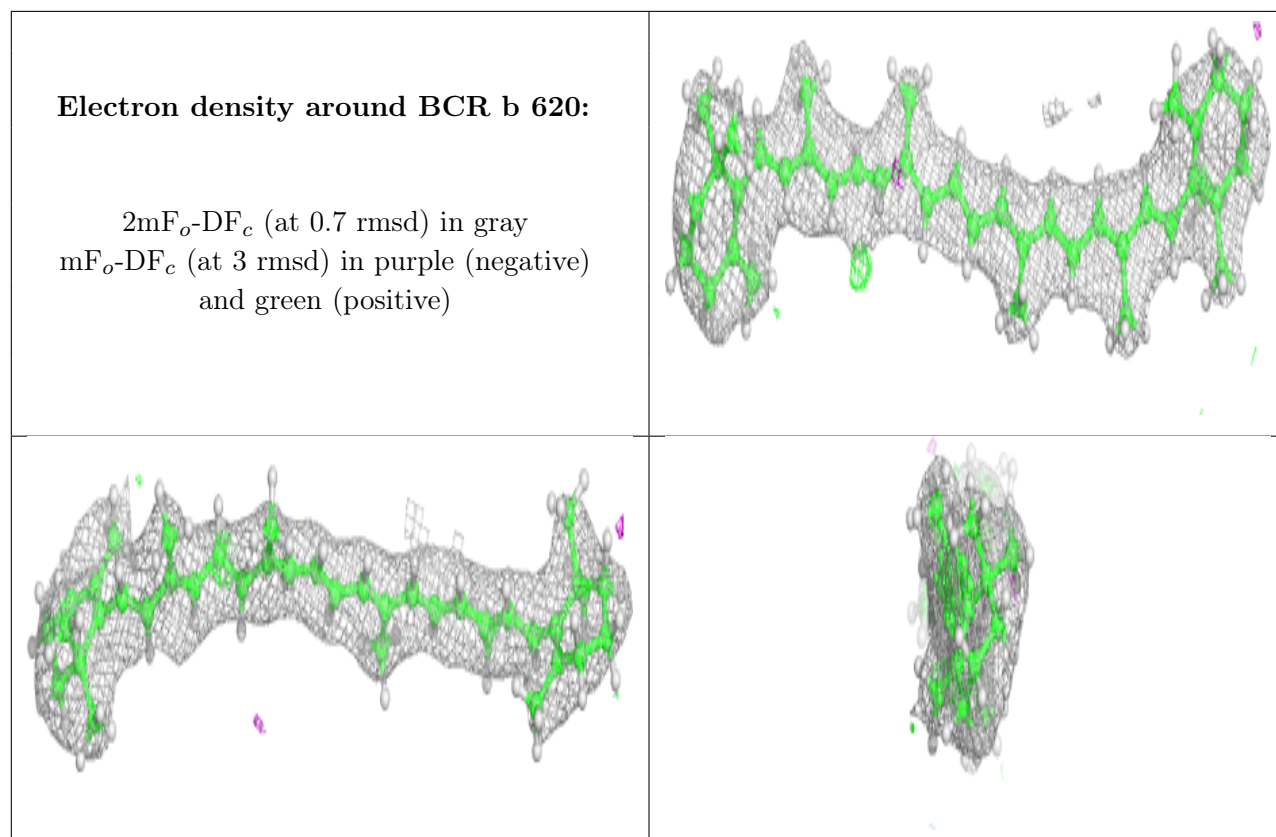
Electron density around BCR b 619:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around LMG B 621:**

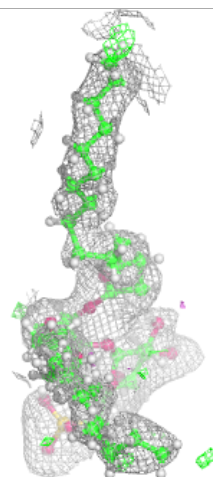
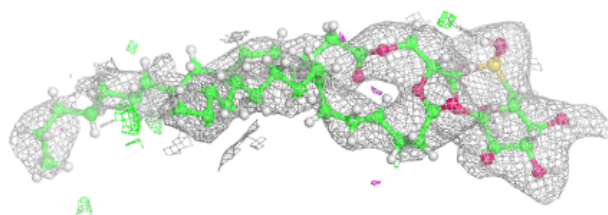
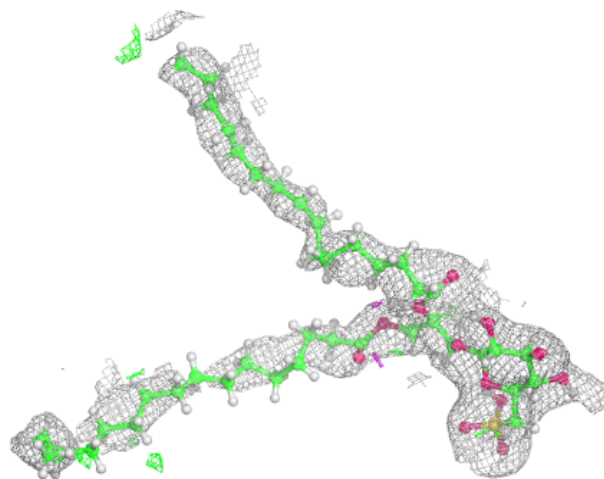
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





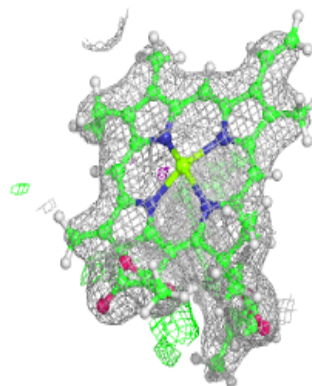
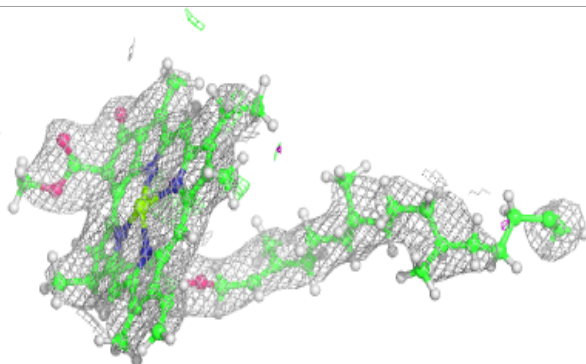
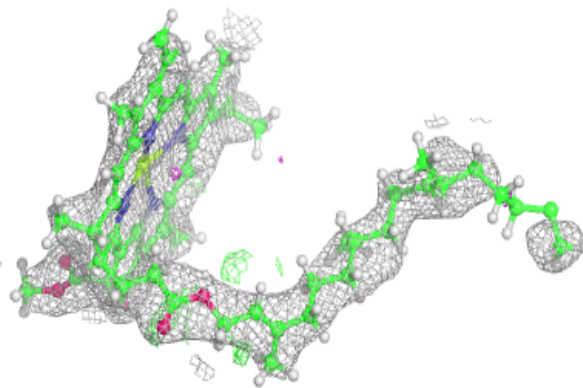
Electron density around SQD a 410:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

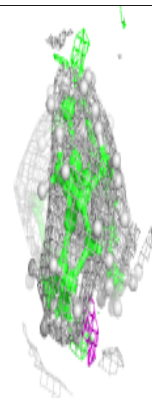
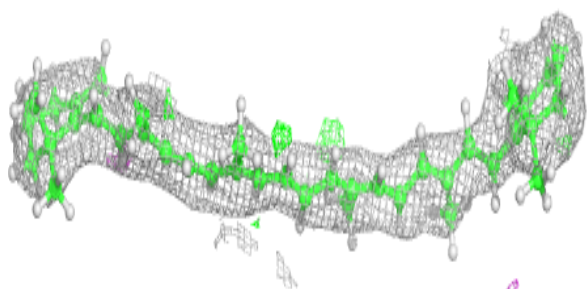
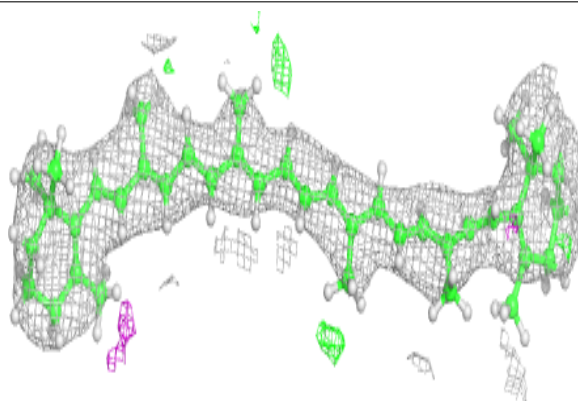


Electron density around CLA c 508:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

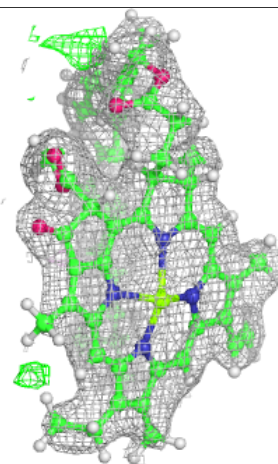
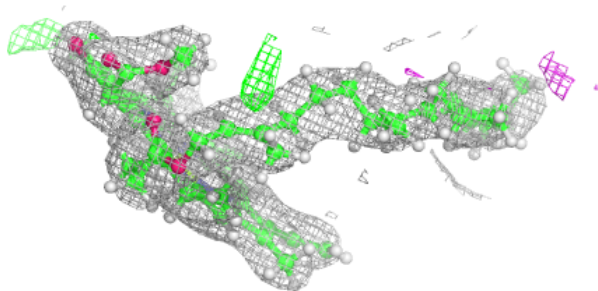
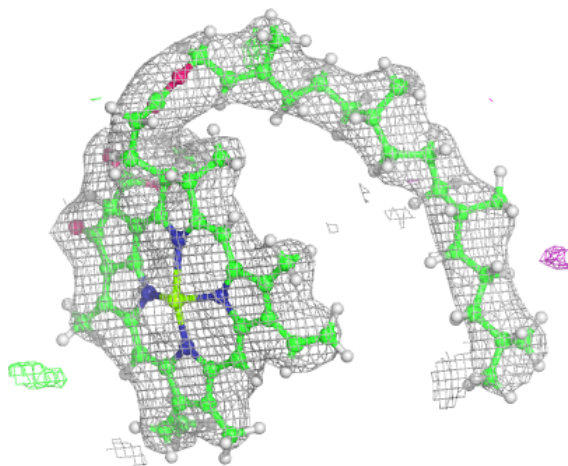
**Electron density around BCR d 406:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



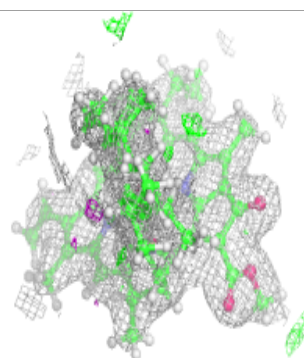
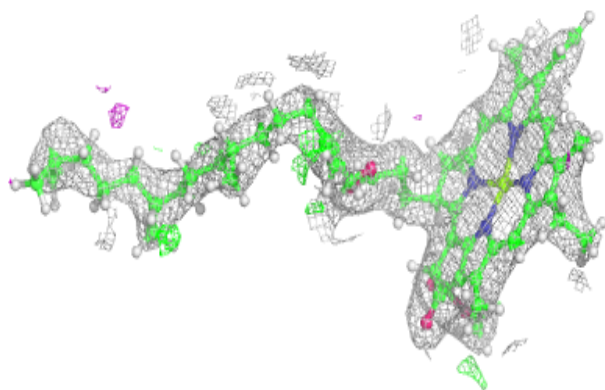
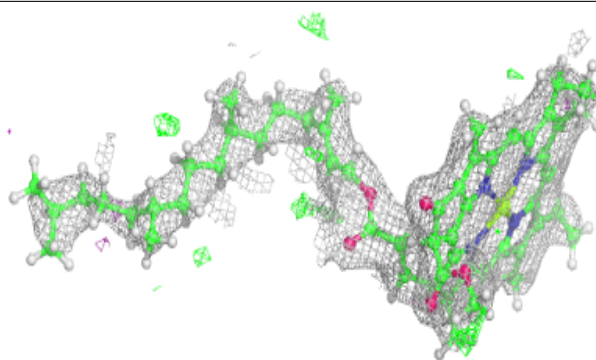
Electron density around CLA C 508:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

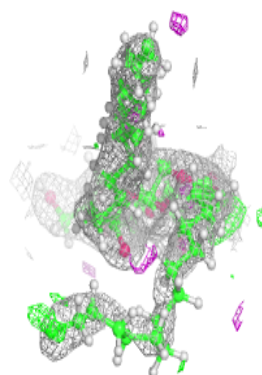
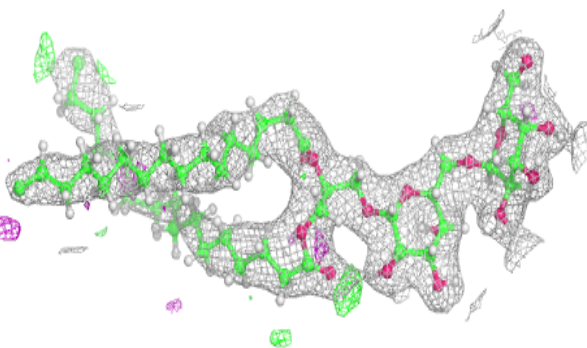
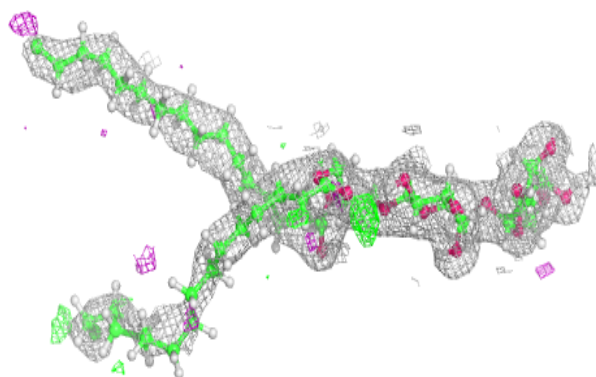


Electron density around CLA c 502:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

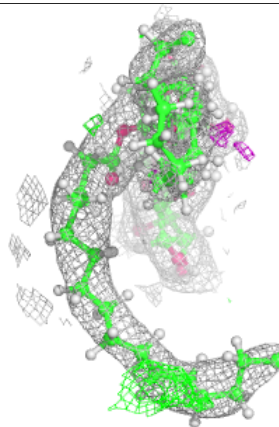
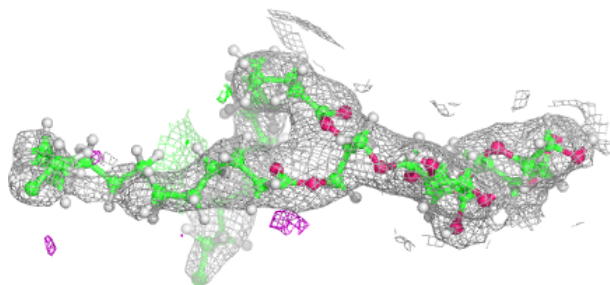
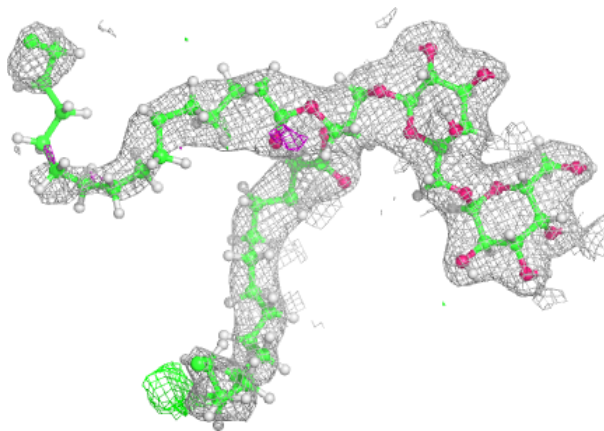
**Electron density around DGD C 516:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



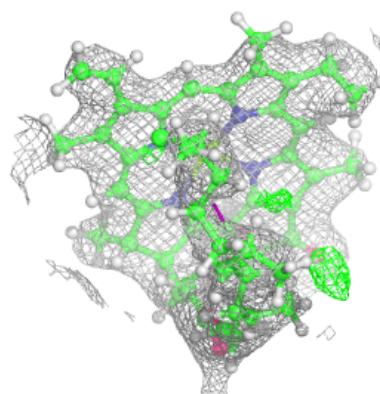
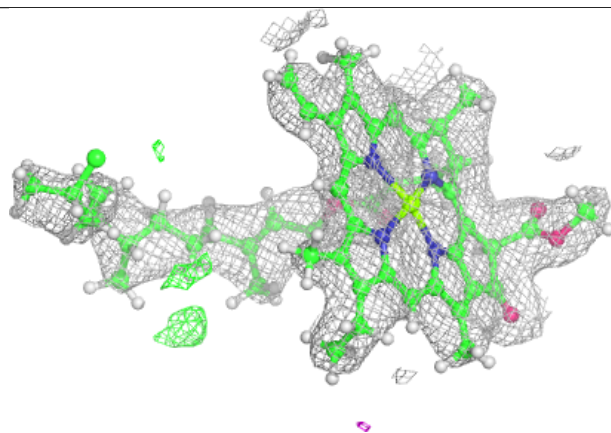
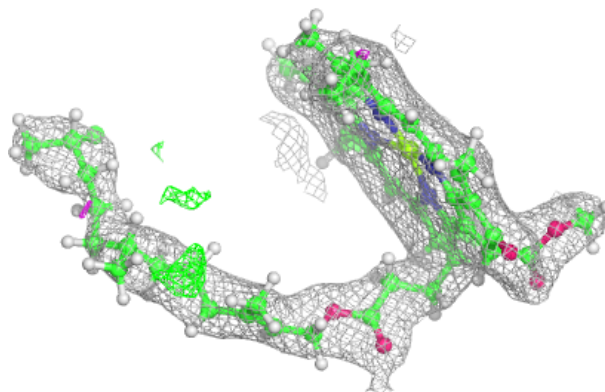
Electron density around DGD C 517:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

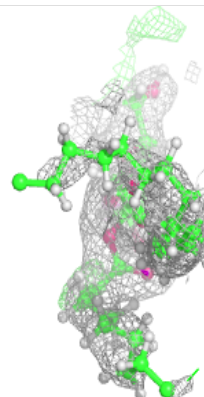
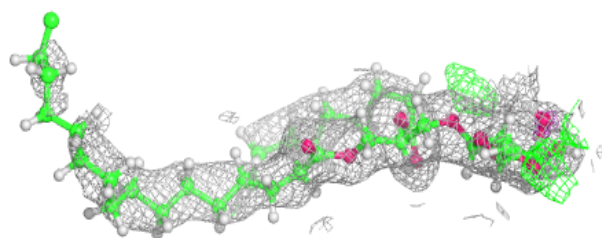
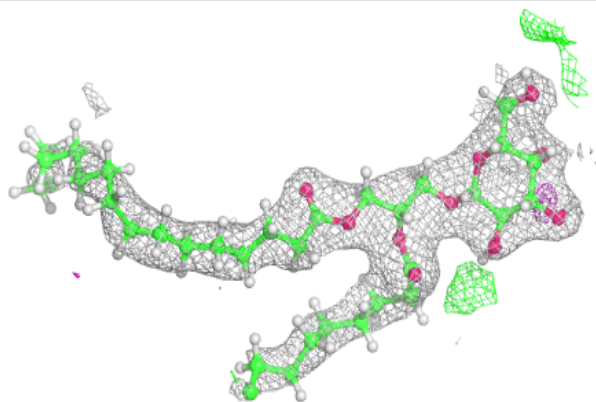


Electron density around CLA c 504:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

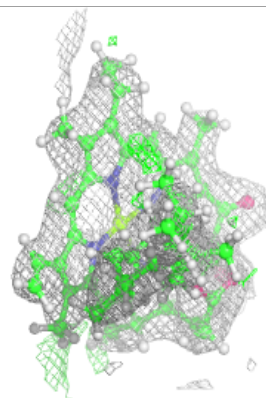
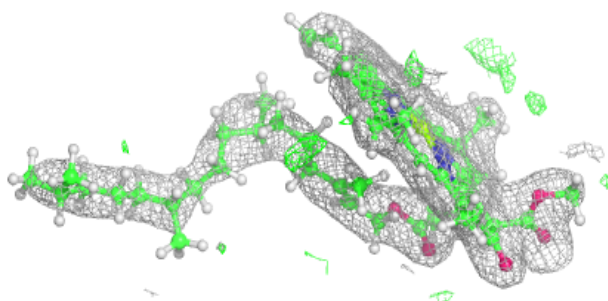
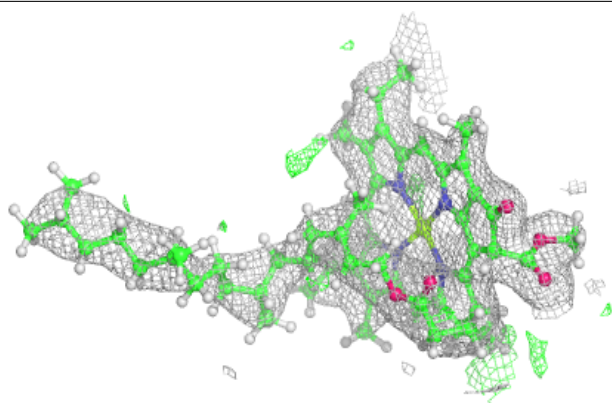
**Electron density around LMG d 411:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

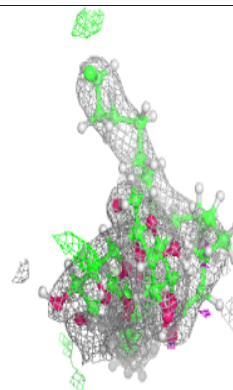
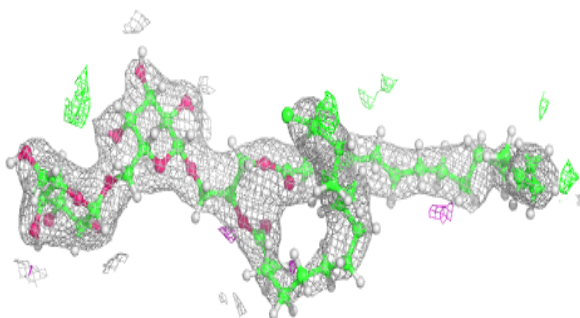
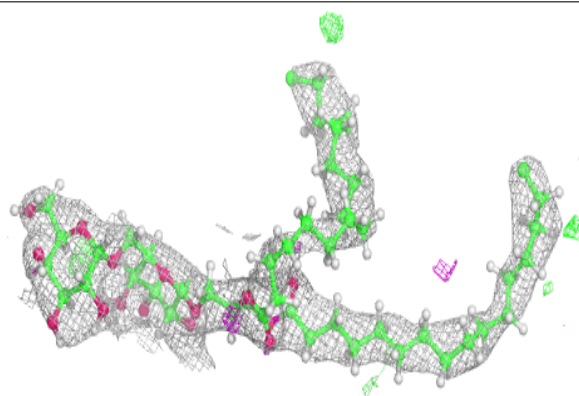


Electron density around CLA C 506:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

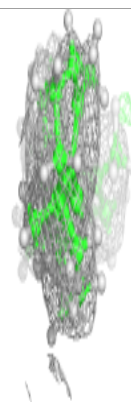
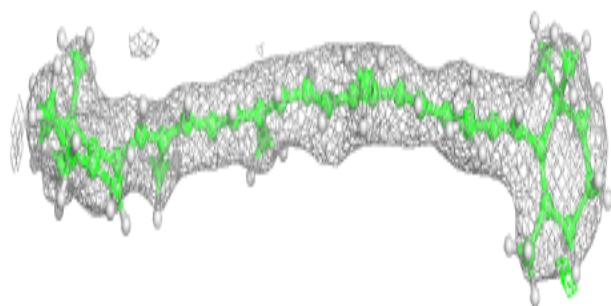
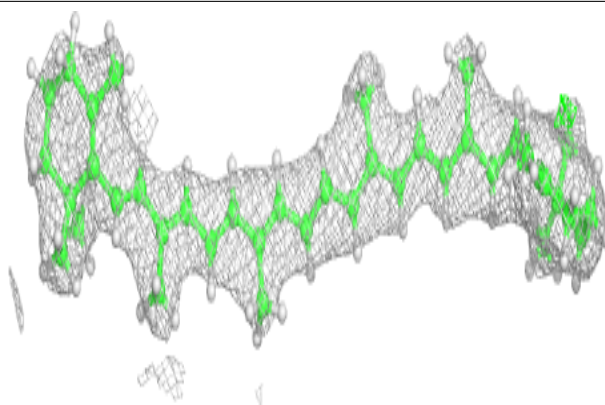
**Electron density around DGD h 104:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

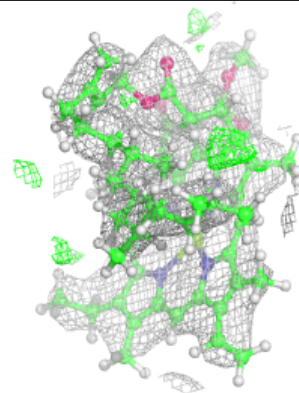
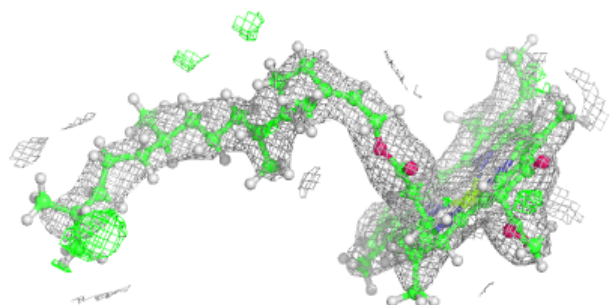
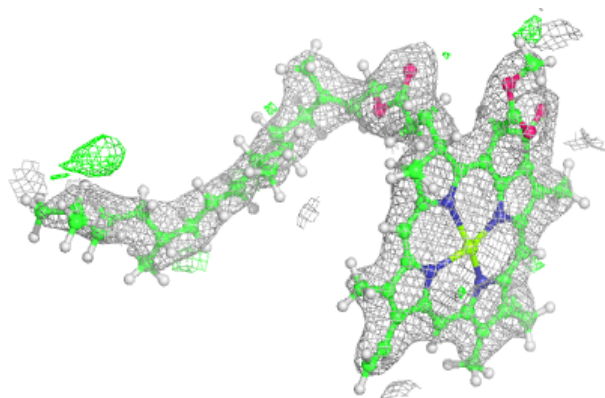


Electron density around BCR b 618:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

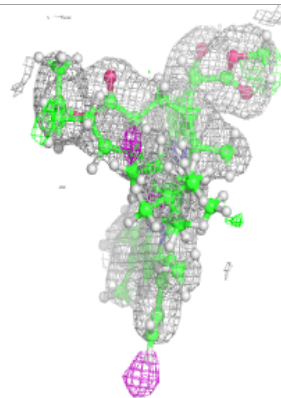
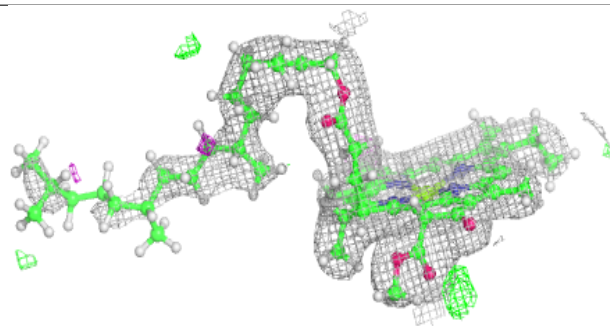
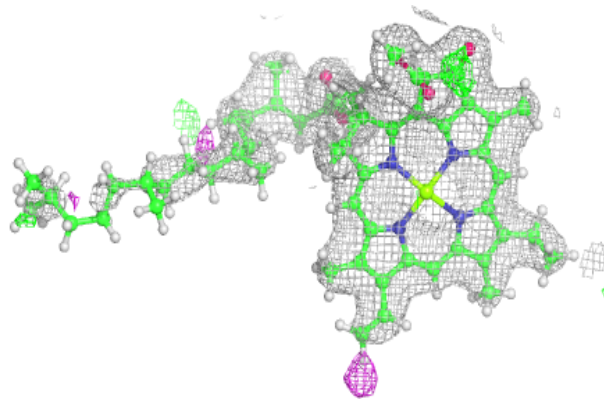
**Electron density around CLA c 511:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

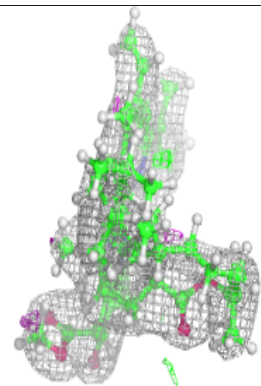
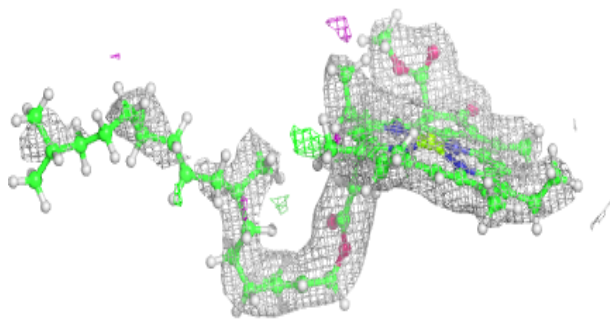
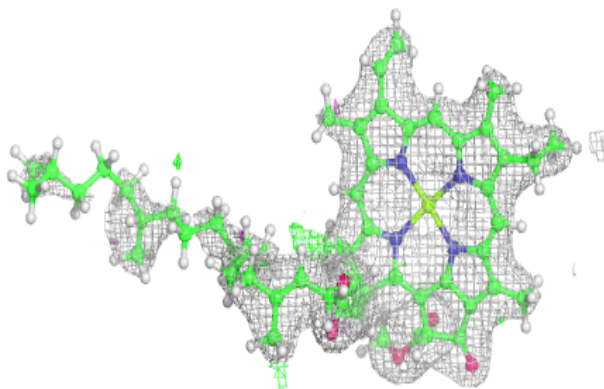


Electron density around CLA A 406:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

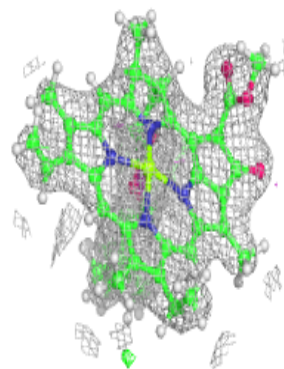
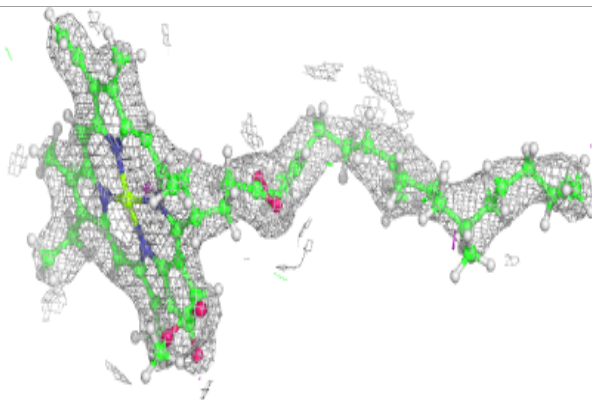
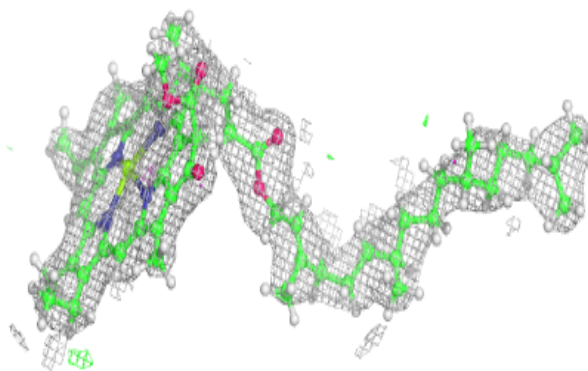
**Electron density around CLA a 405:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

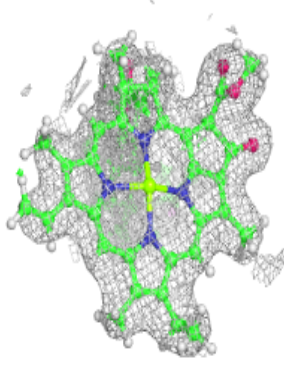
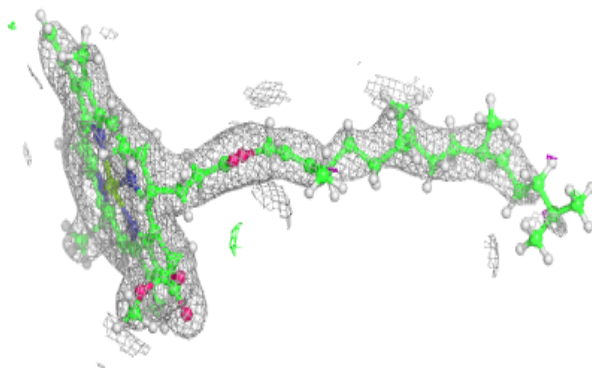
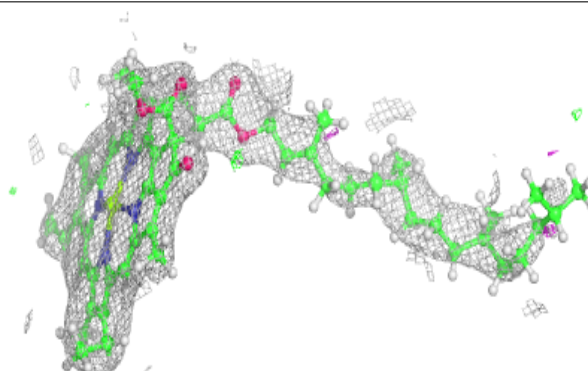


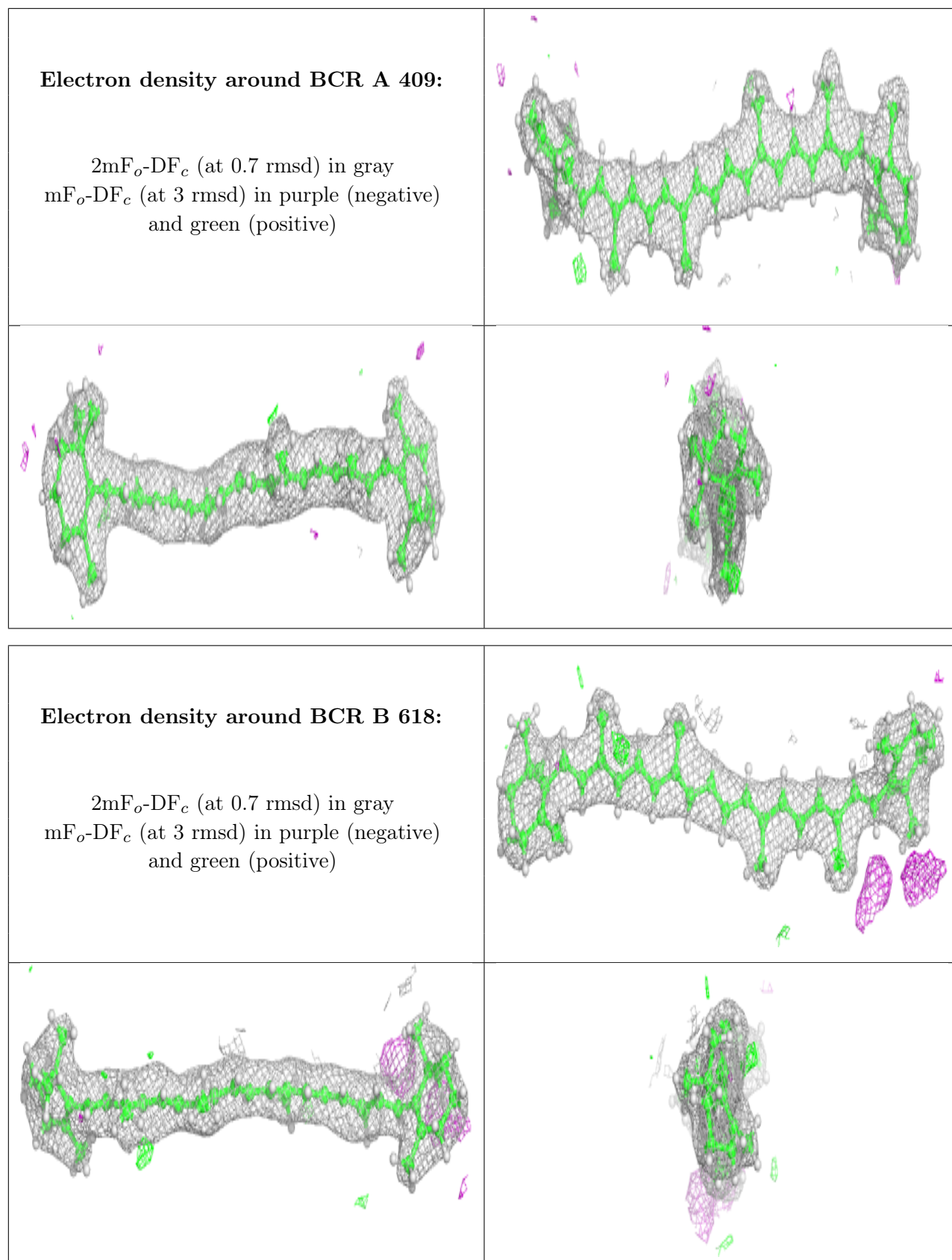
Electron density around CLA C 503:

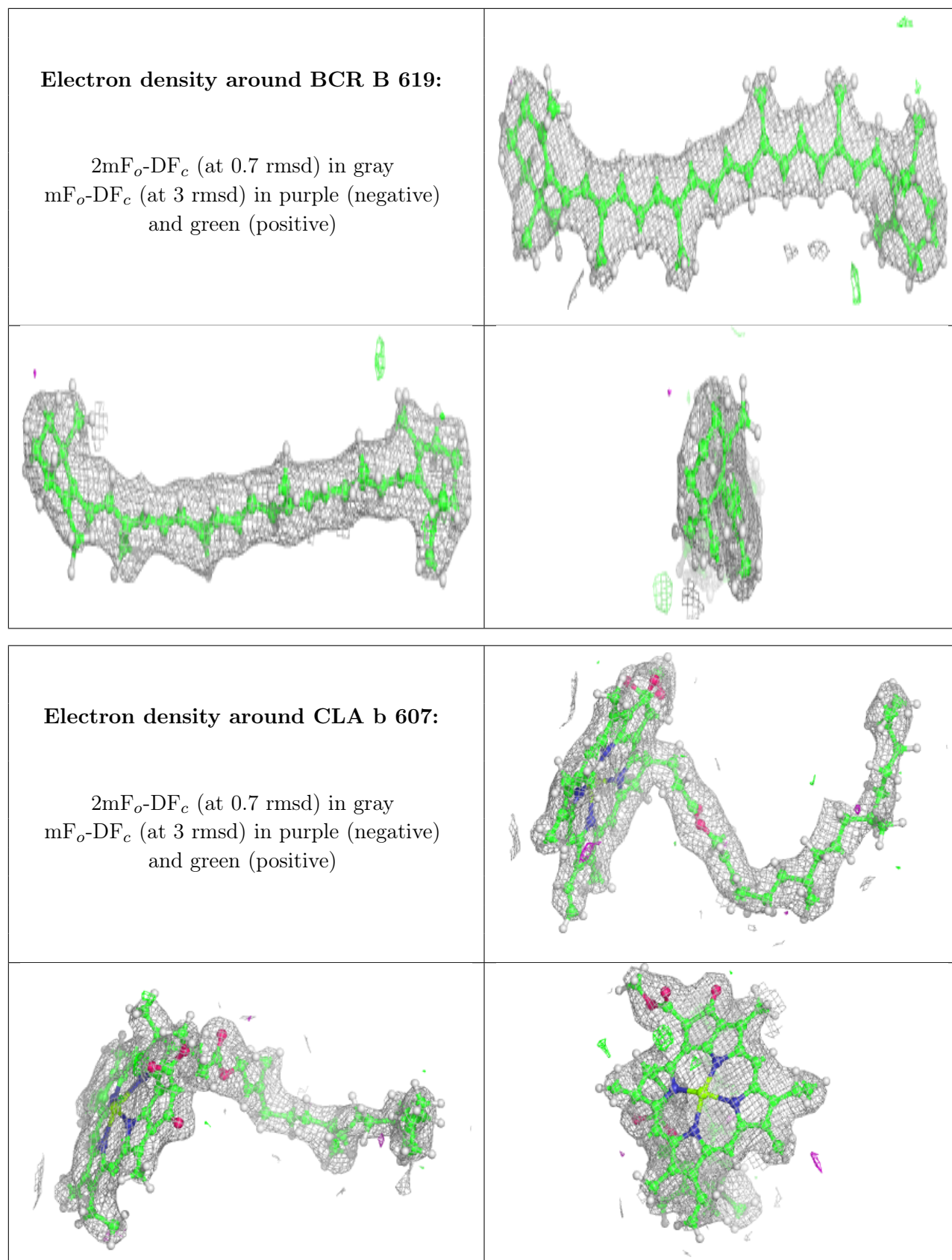
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

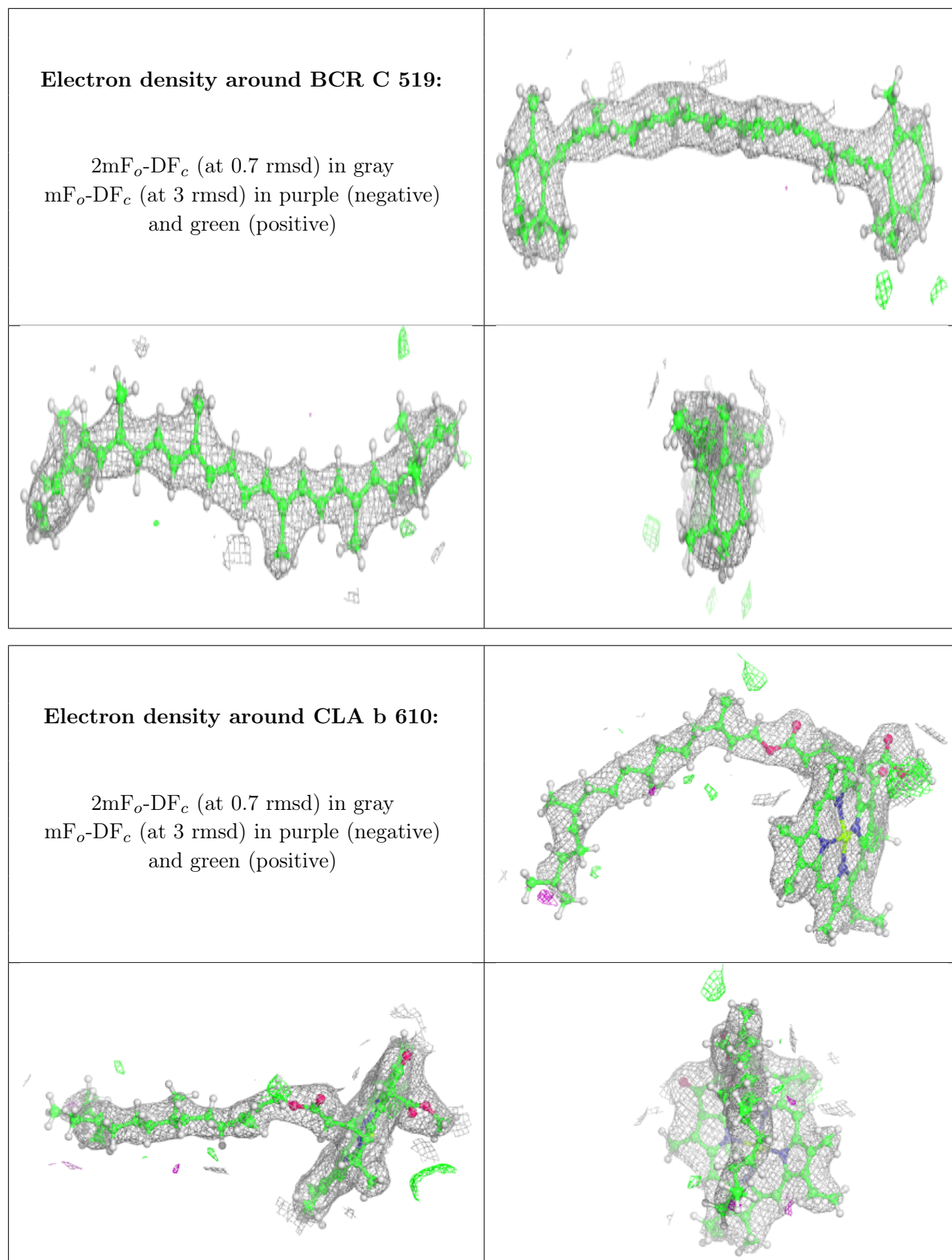
**Electron density around CLA b 605:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



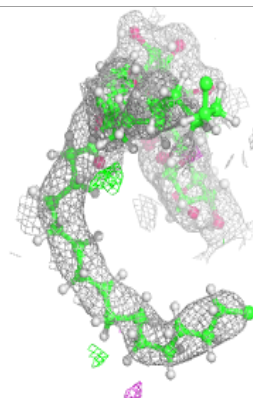
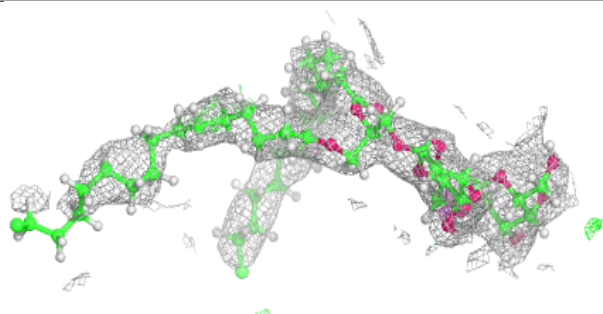
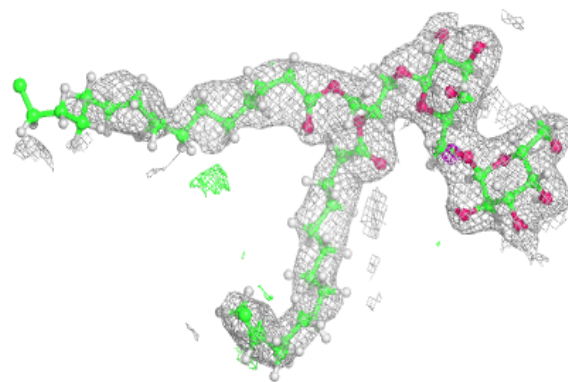




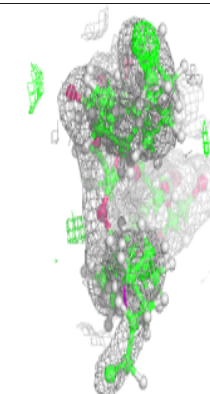
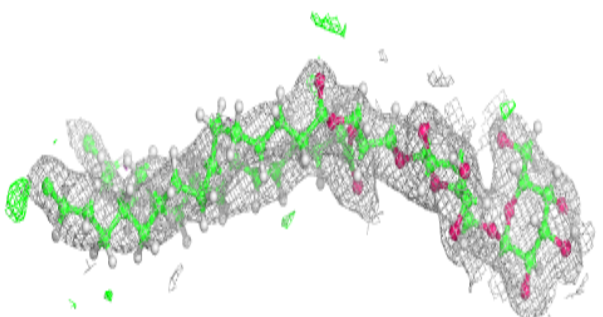
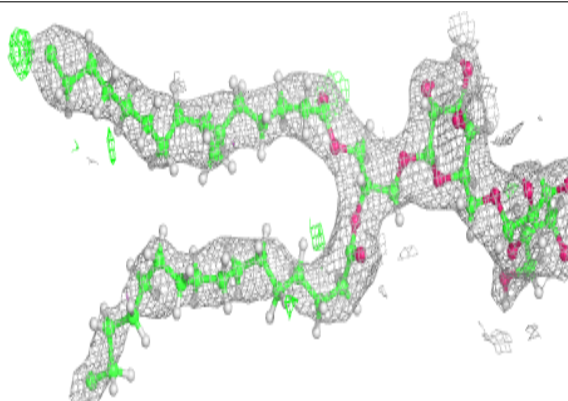


Electron density around DGD c 517:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

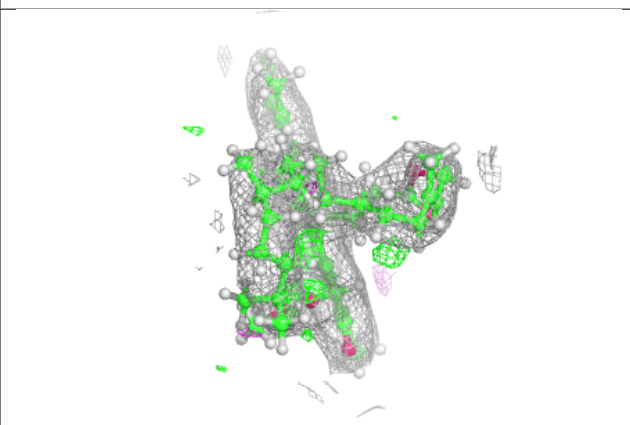
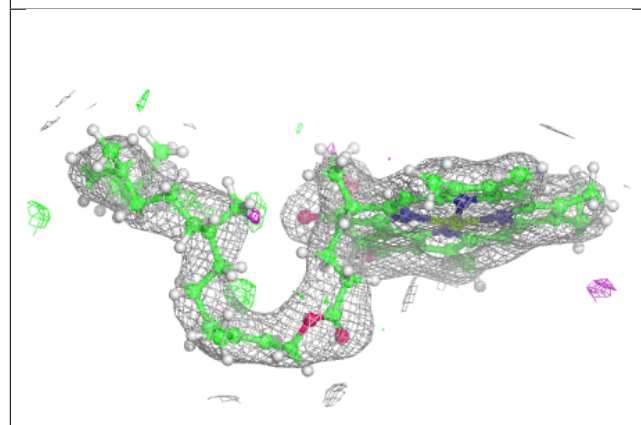
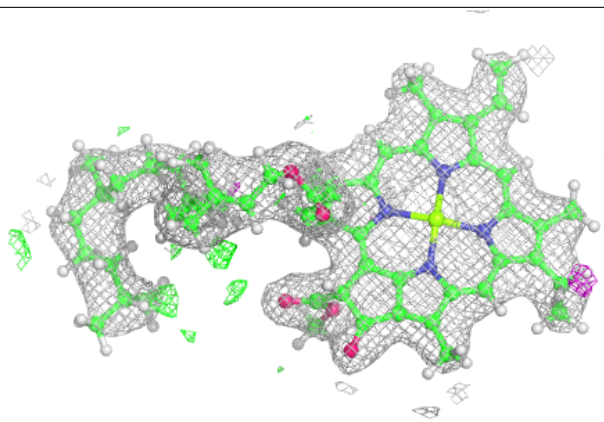
**Electron density around DGD c 518:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

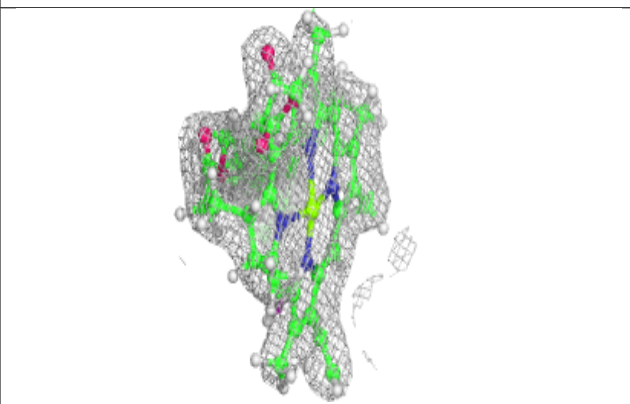
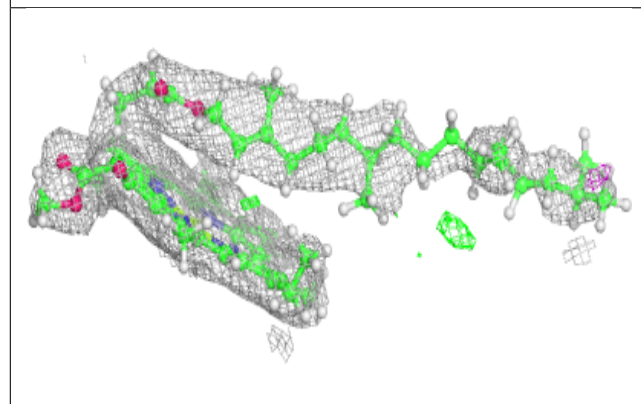
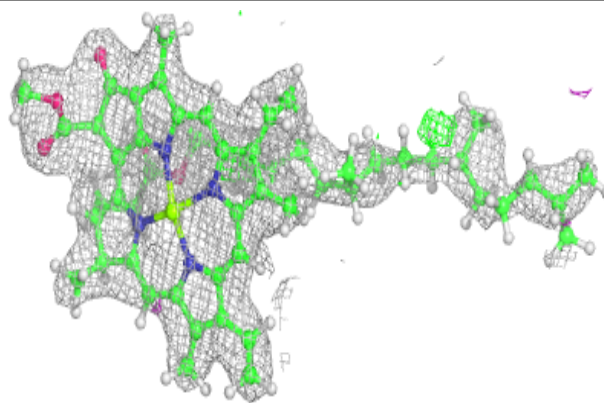


Electron density around CLA b 613:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

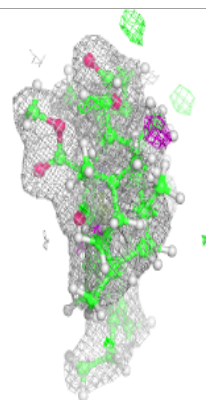
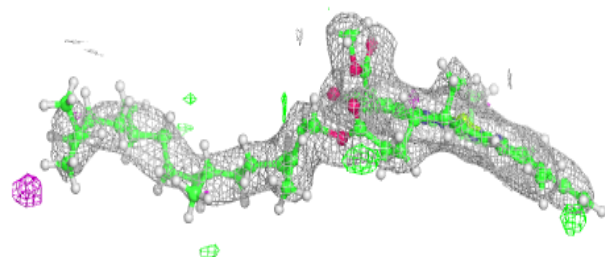
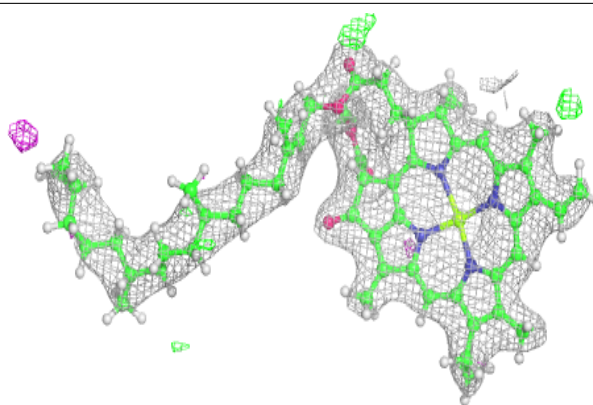
**Electron density around CLA b 615:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

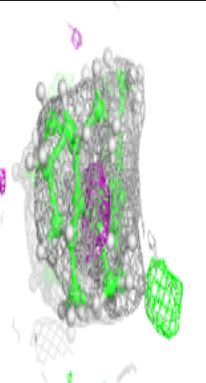
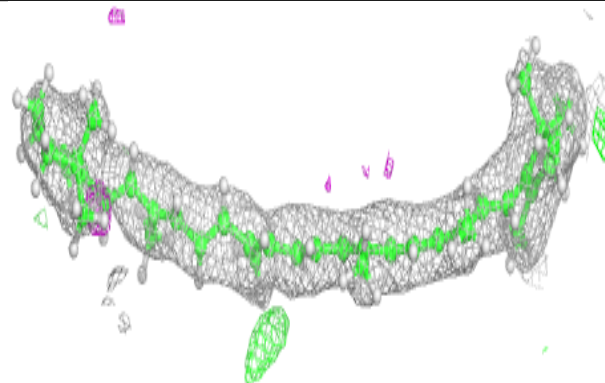
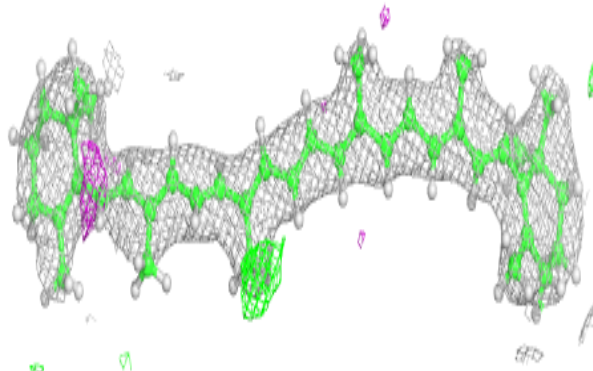


Electron density around CLA B 602:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

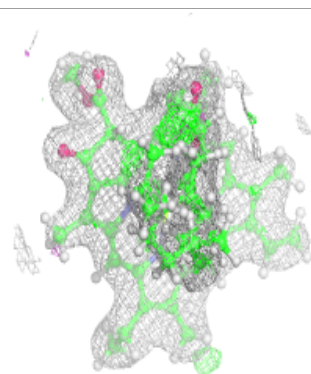
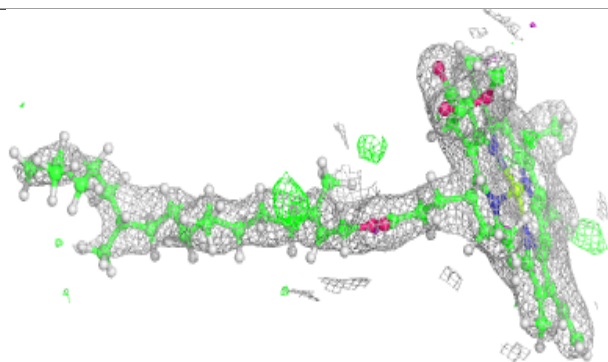
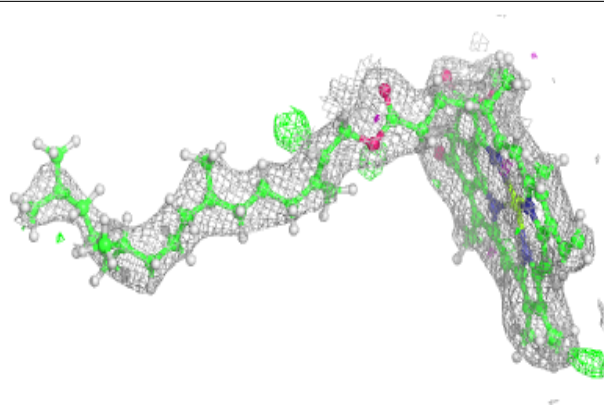
**Electron density around BCR b 602:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



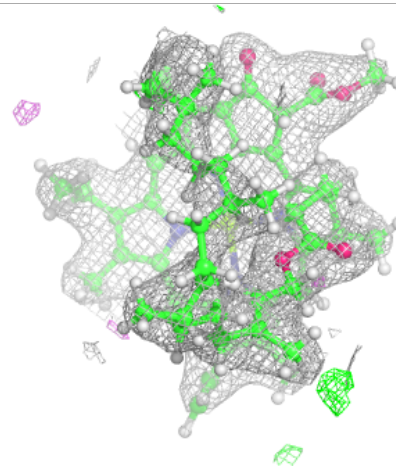
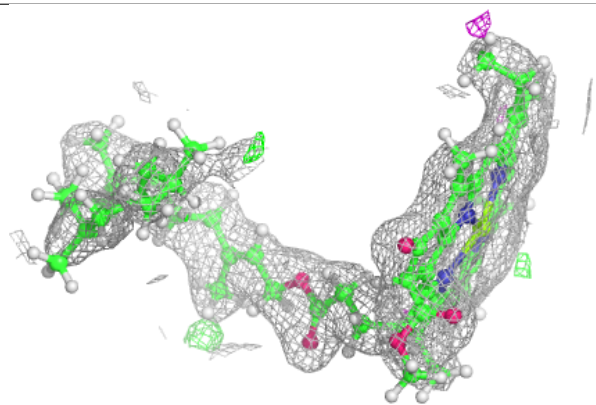
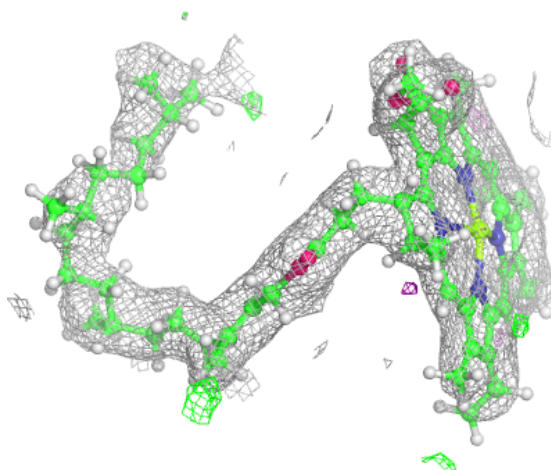
Electron density around CLA B 604:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



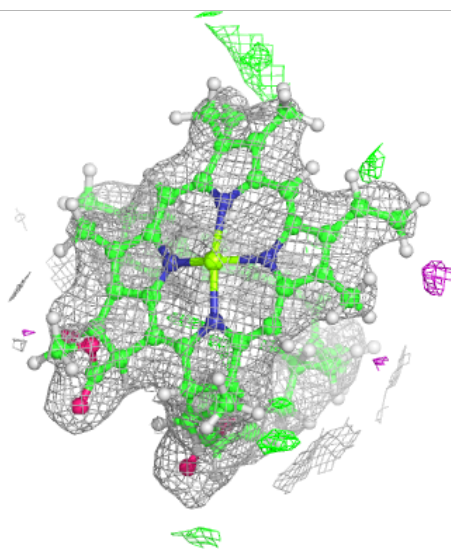
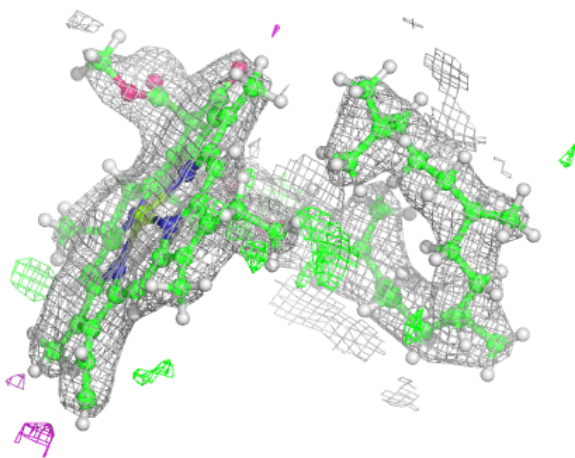
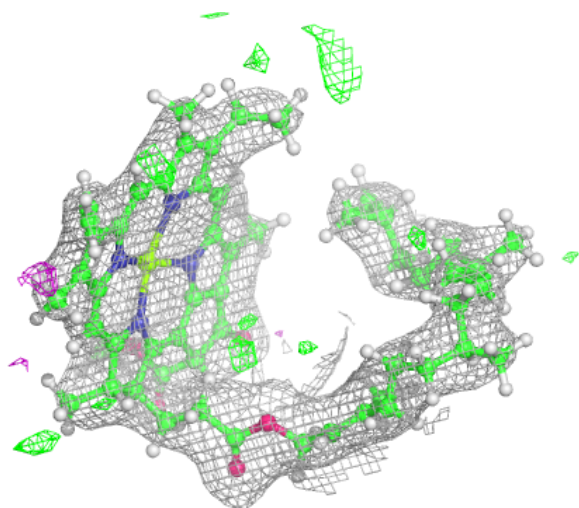
Electron density around CLA B 606:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



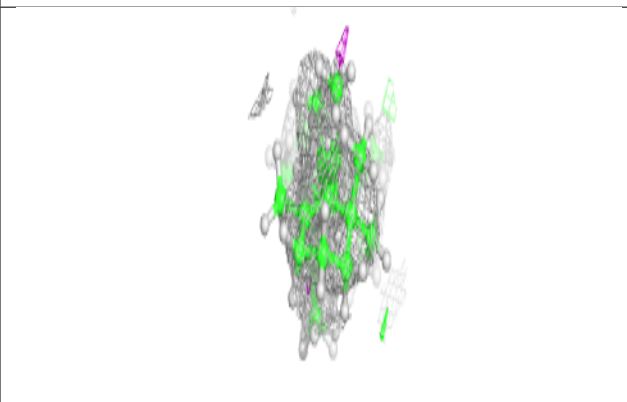
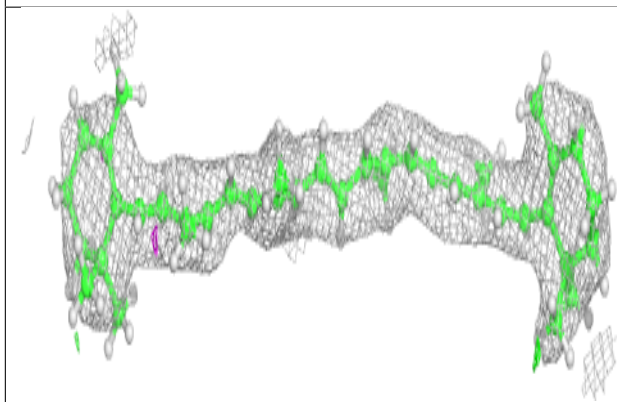
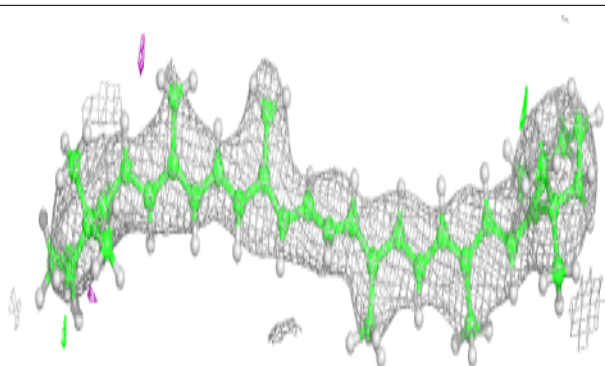
Electron density around CLA c 503:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

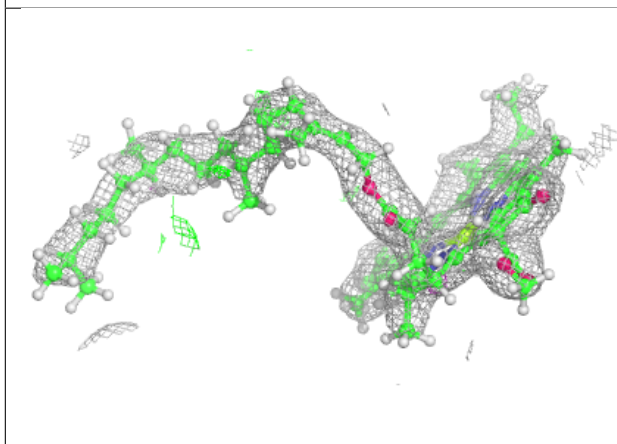
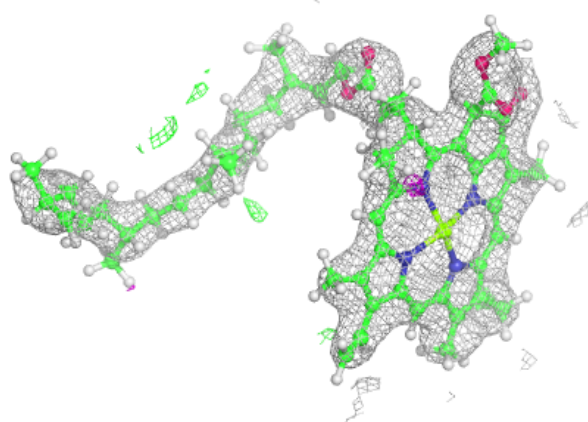


Electron density around BCR c 514:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

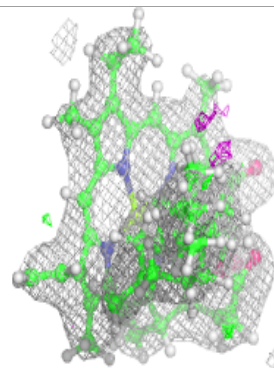
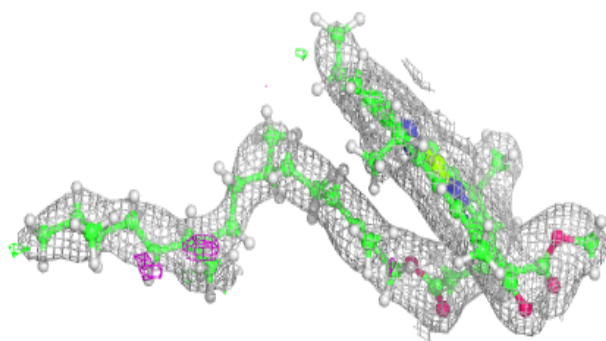
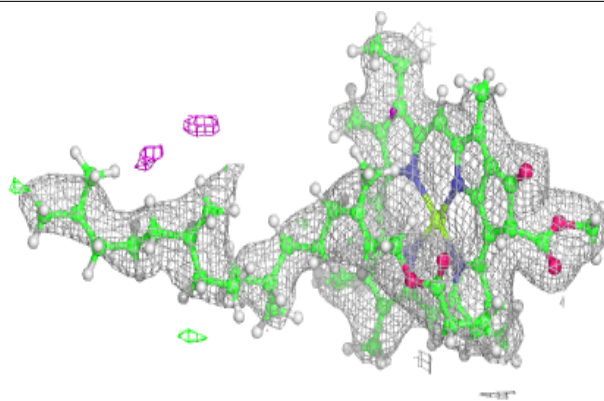
**Electron density around CLA C 512:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



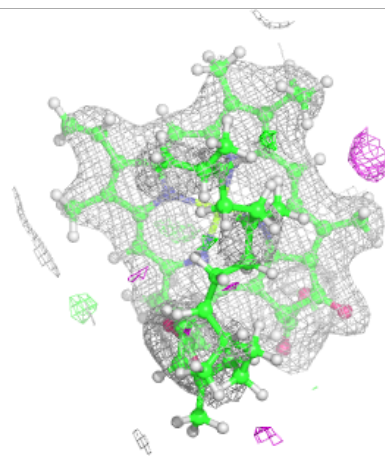
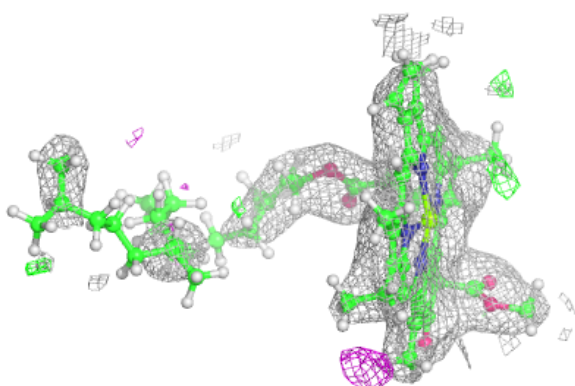
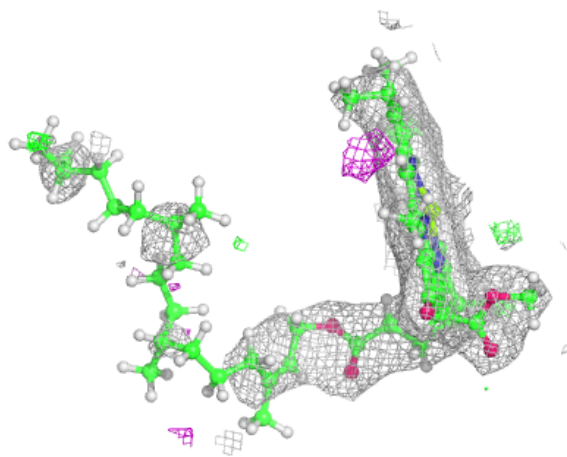
Electron density around CLA c 505:

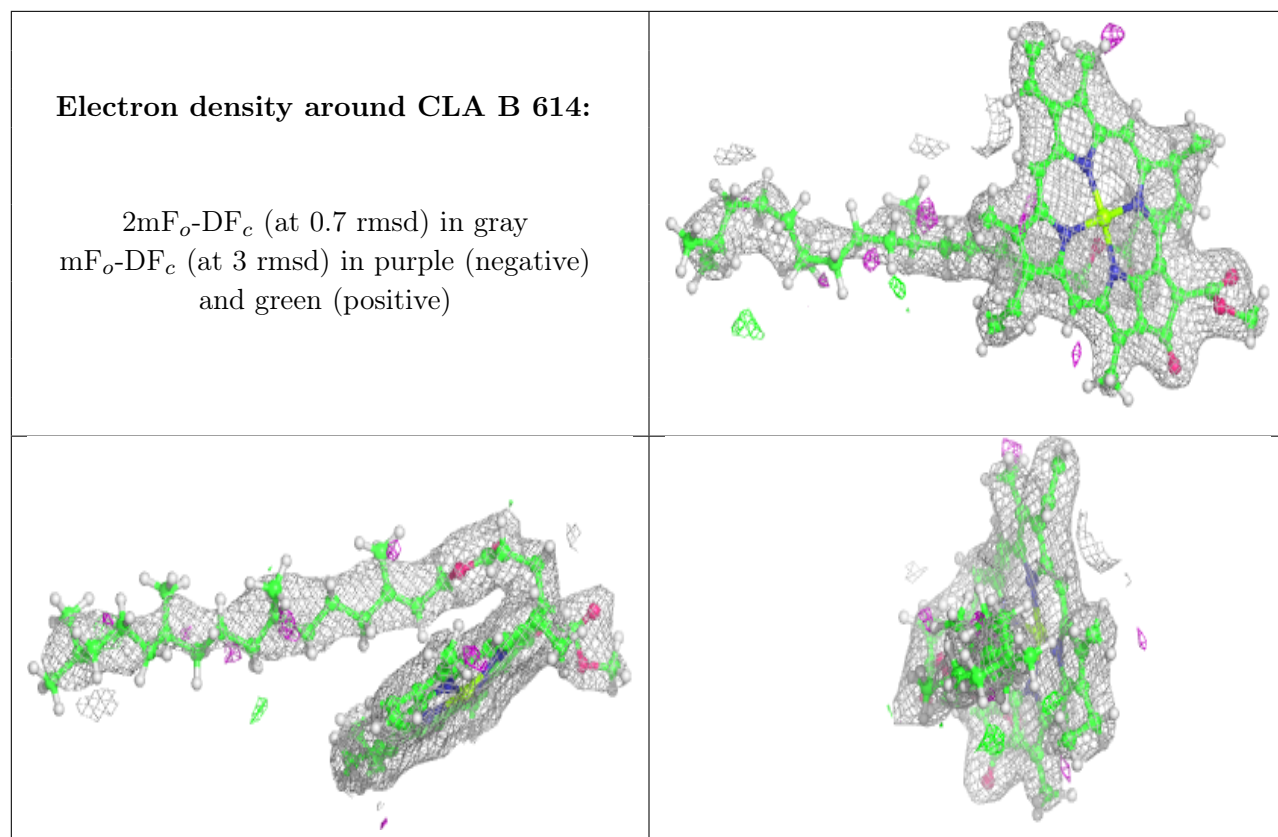
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA c 506:

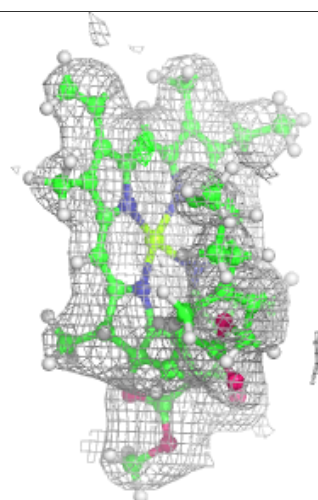
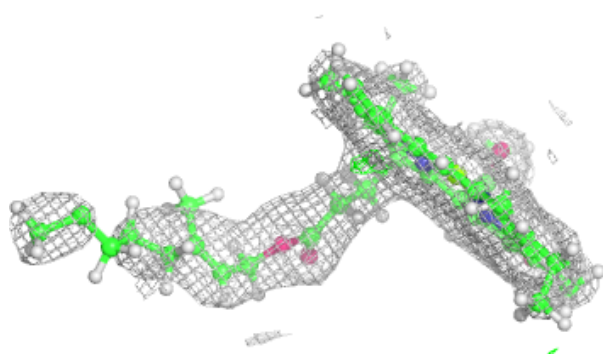
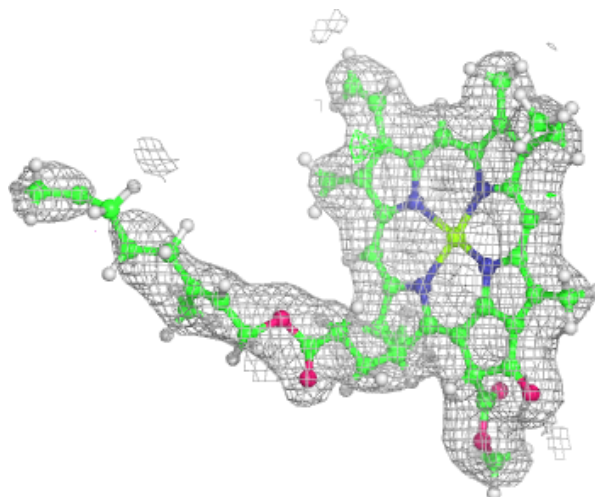
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





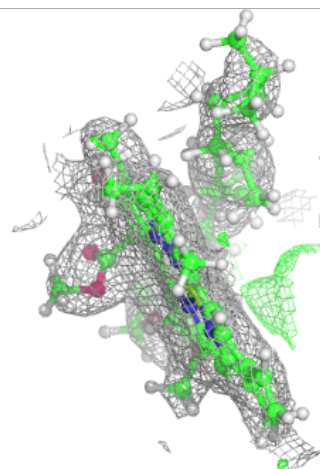
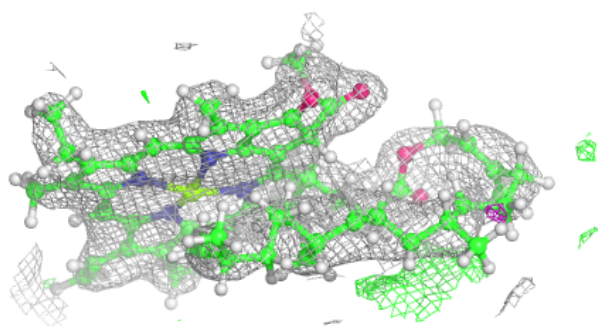
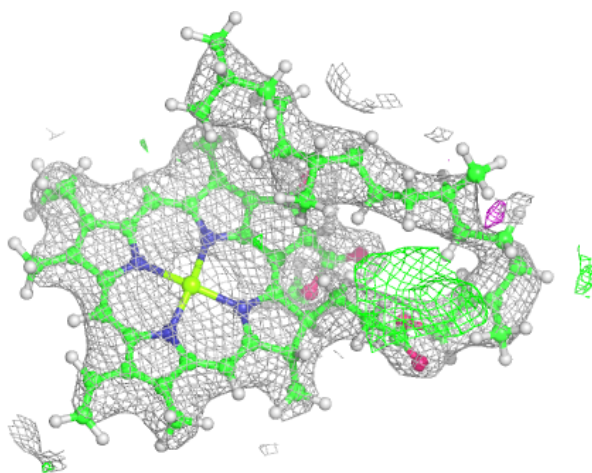
Electron density around CLA A 408:

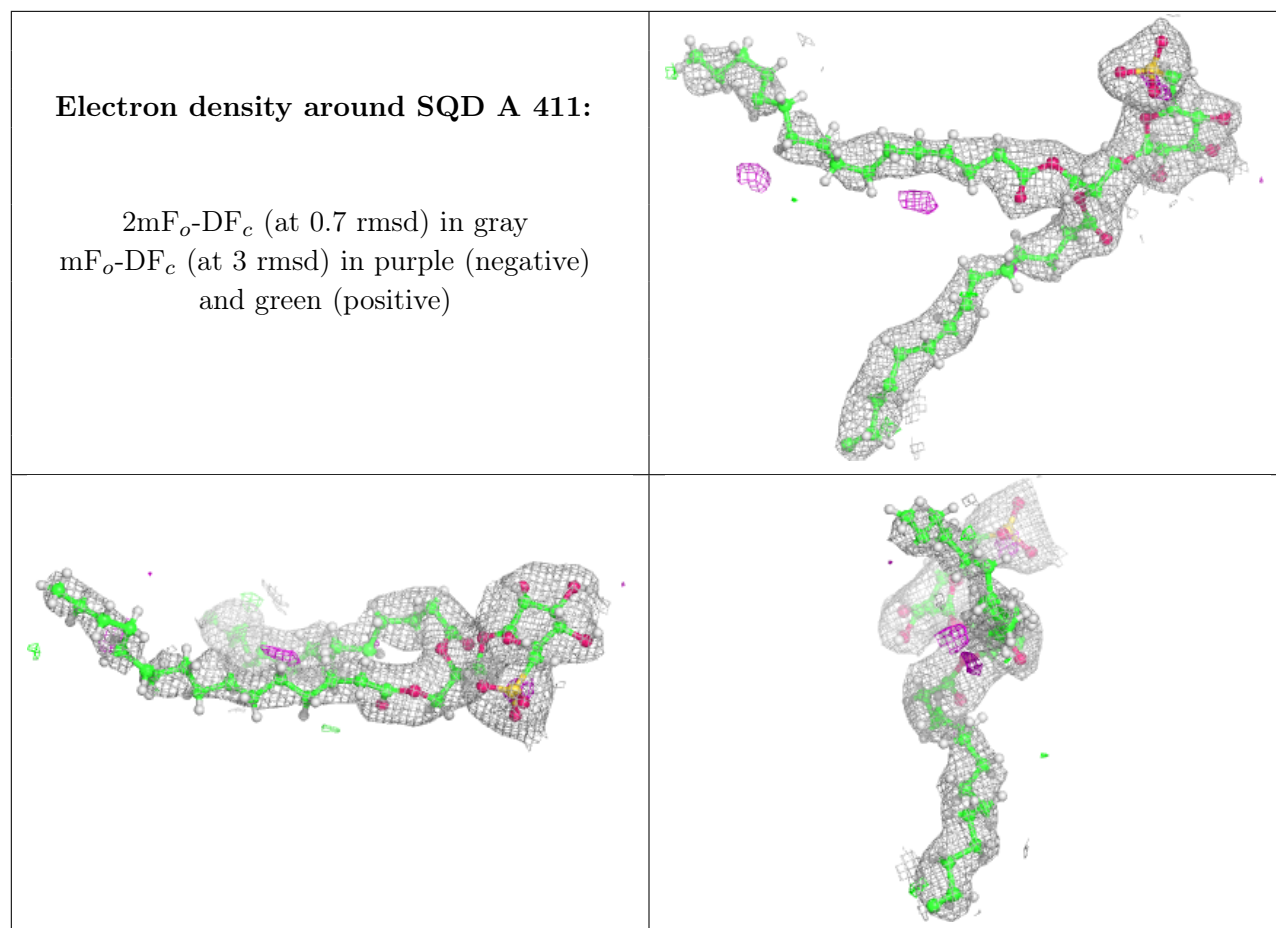
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA c 509:

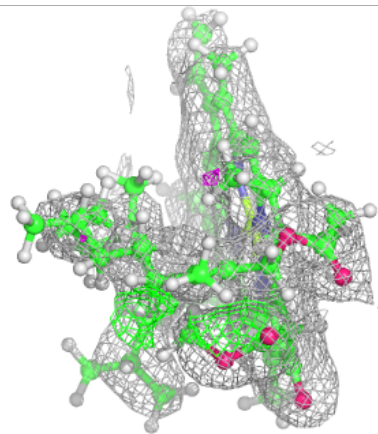
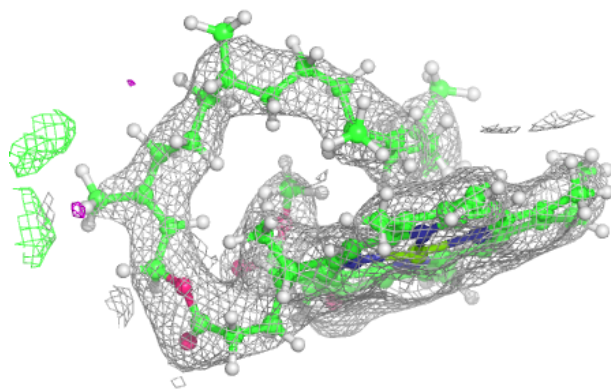
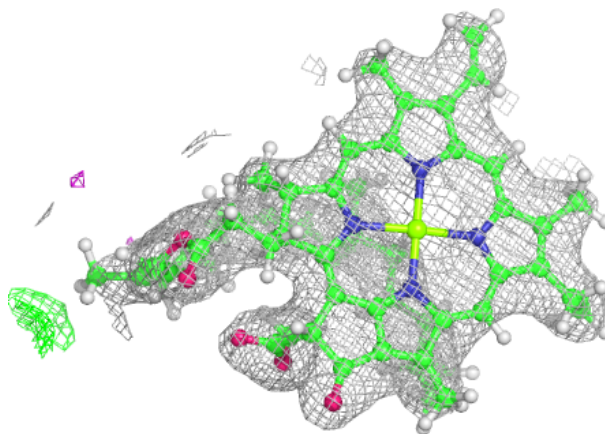
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





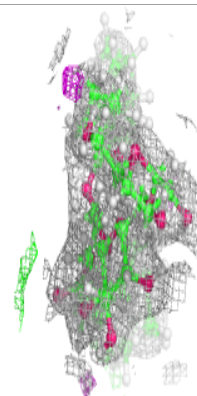
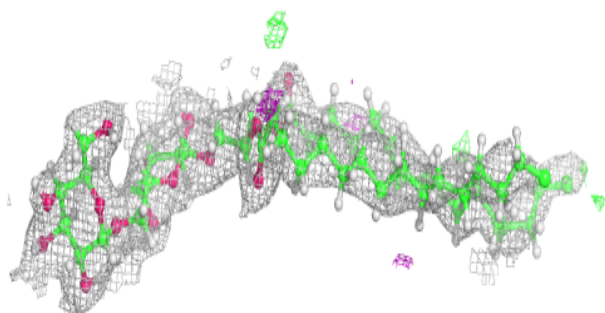
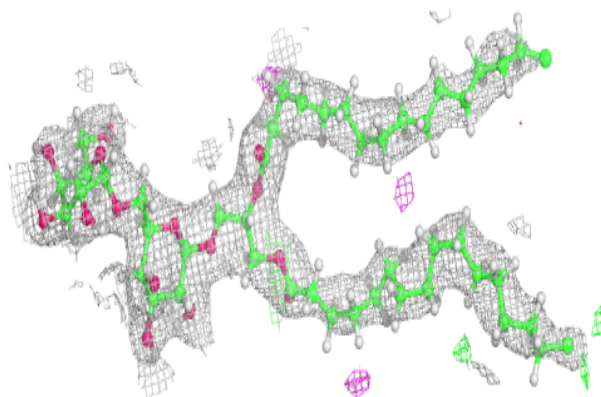
Electron density around CLA c 510:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

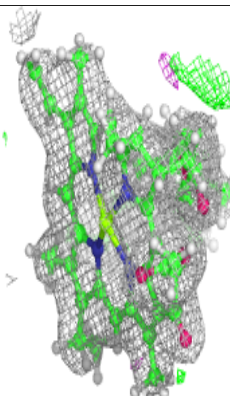
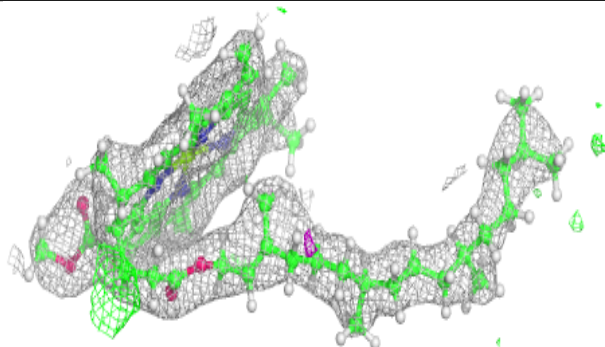
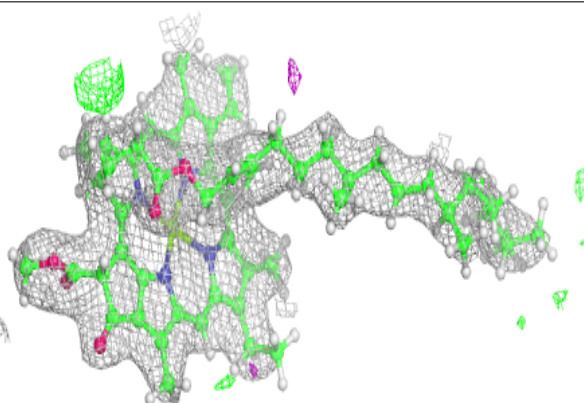


Electron density around DGD C 518:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

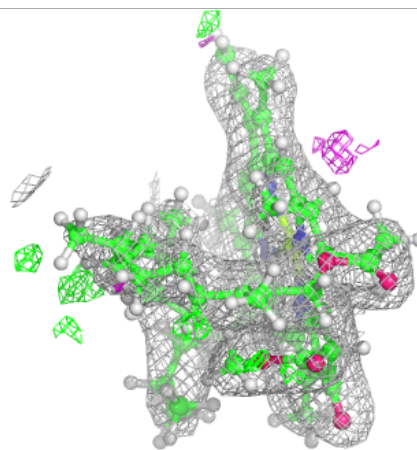
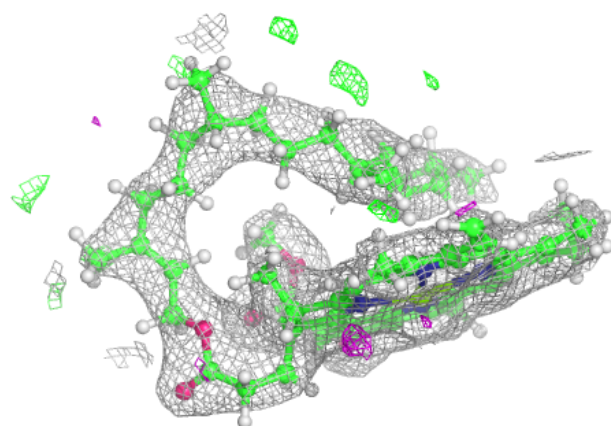
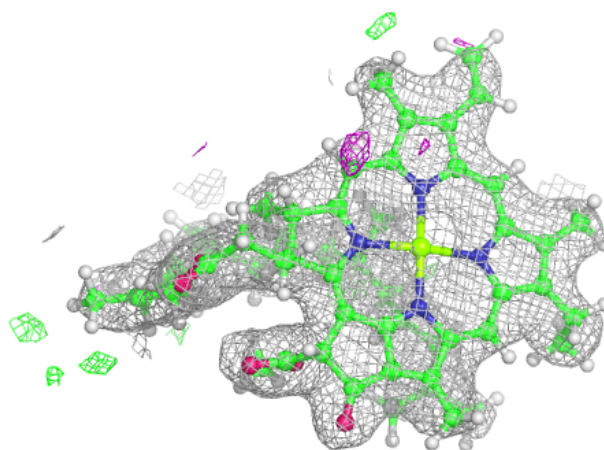
**Electron density around CLA b 609:**

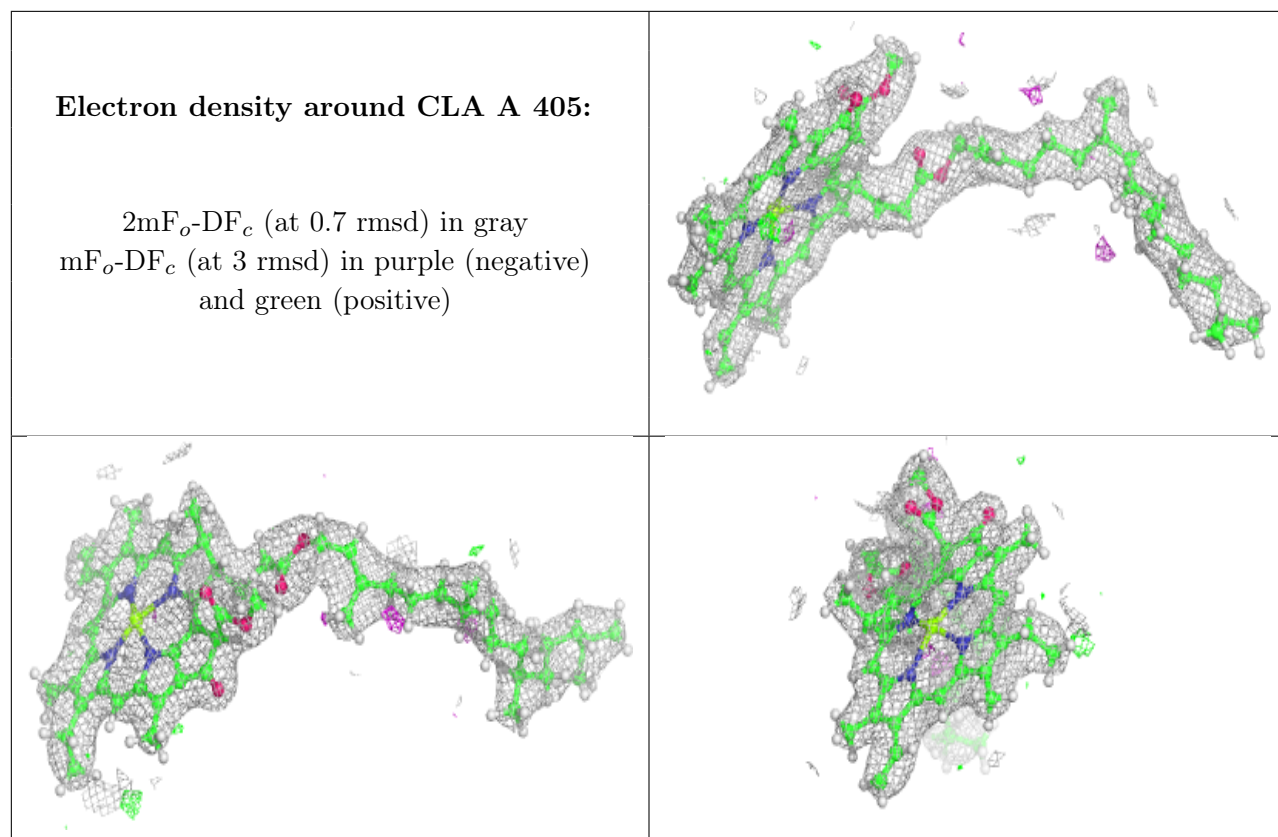
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA C 511:

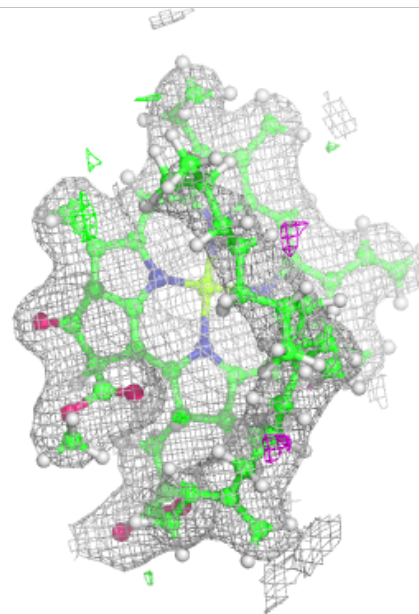
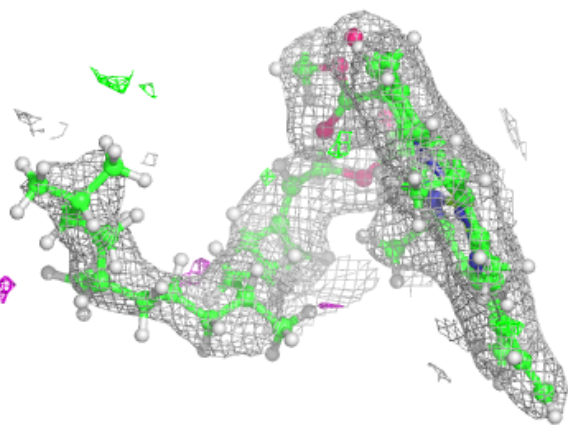
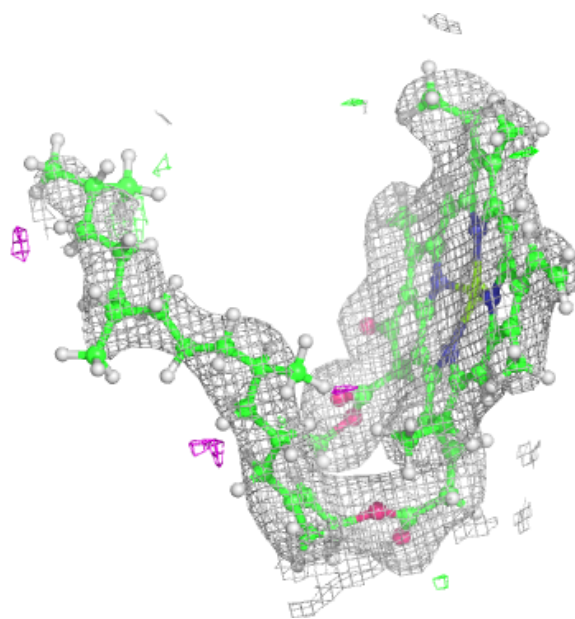
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





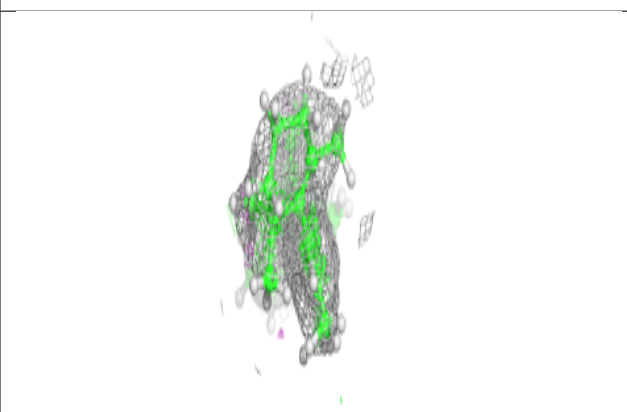
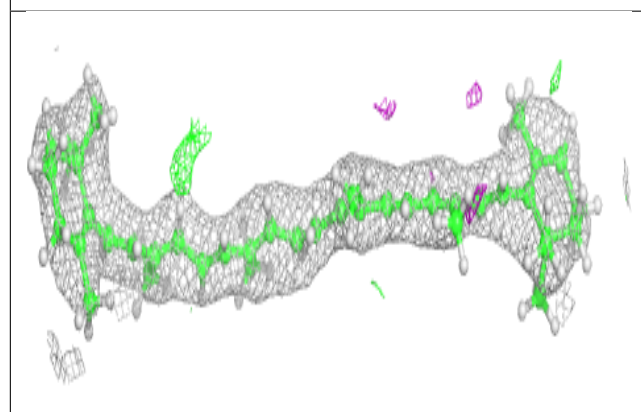
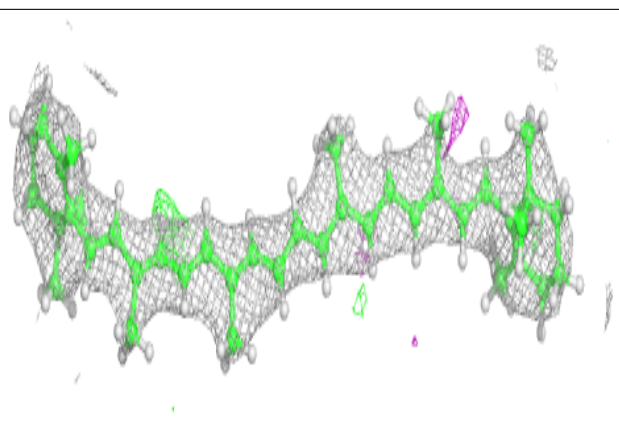
Electron density around CLA b 614:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

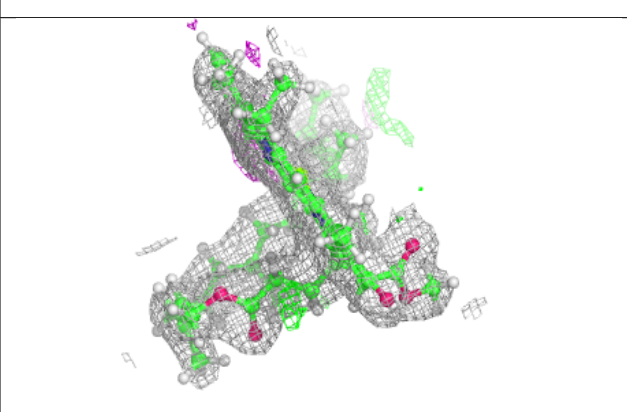
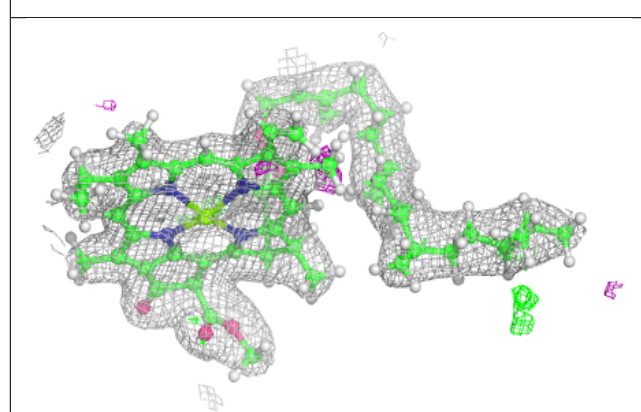
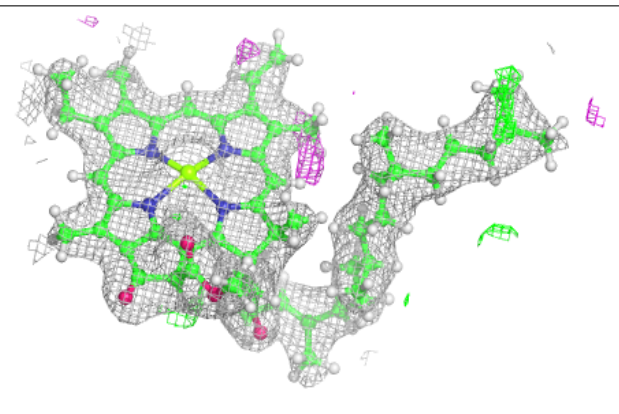


Electron density around BCR c 515:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

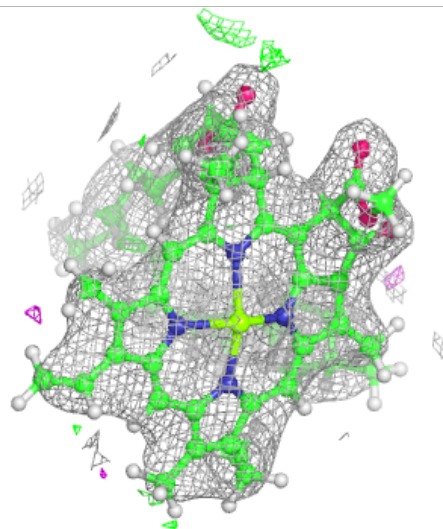
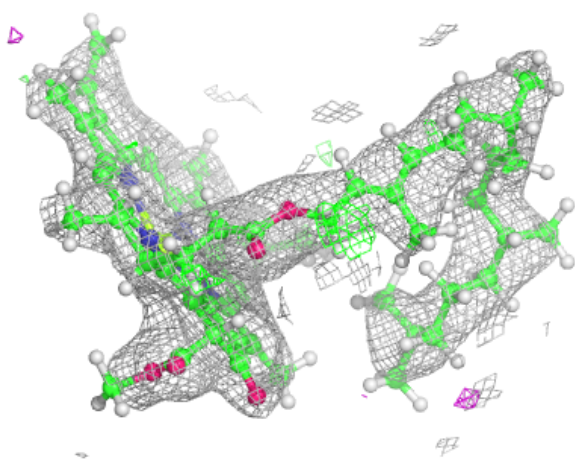
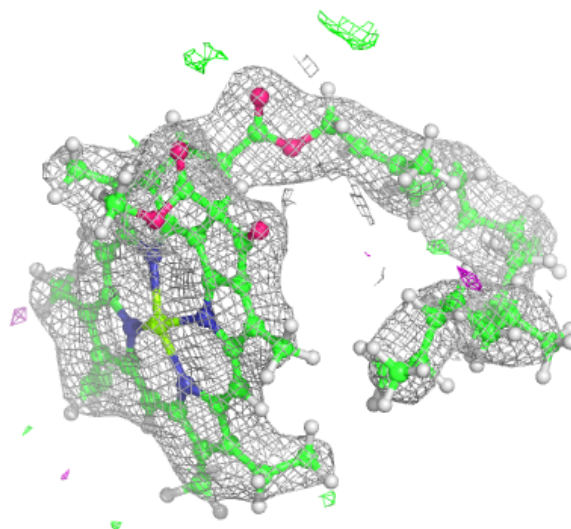
**Electron density around CLA d 403:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



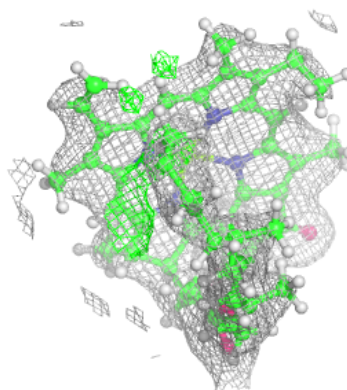
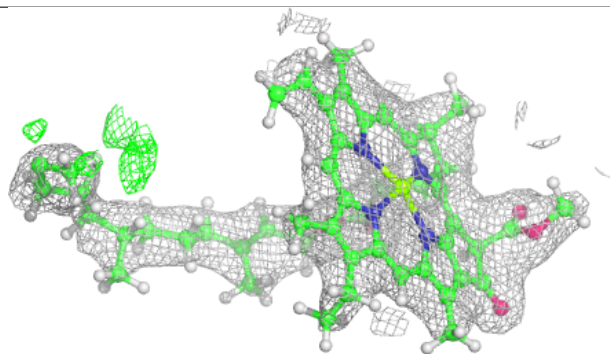
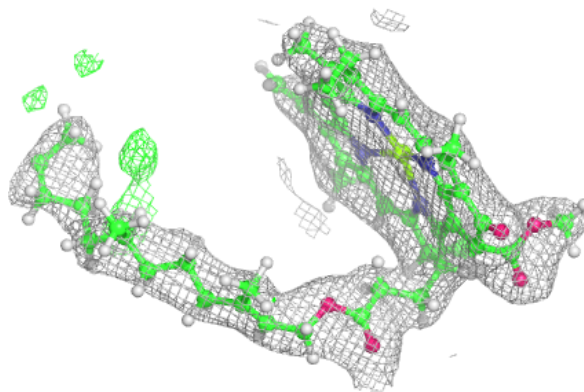
Electron density around CLA C 504:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

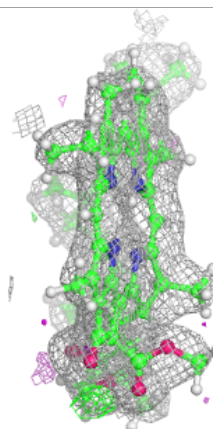
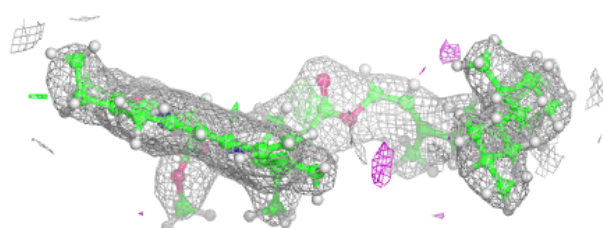
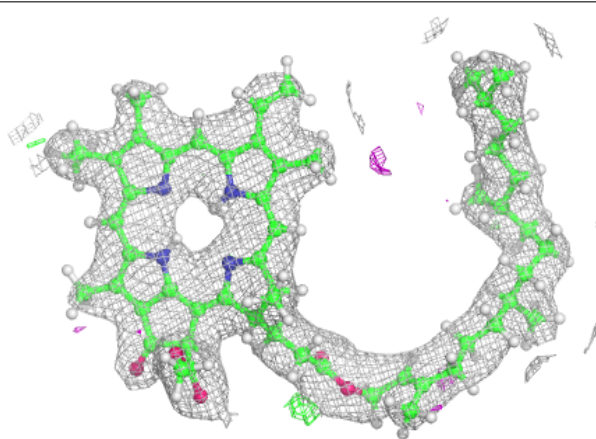


Electron density around CLA C 505:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

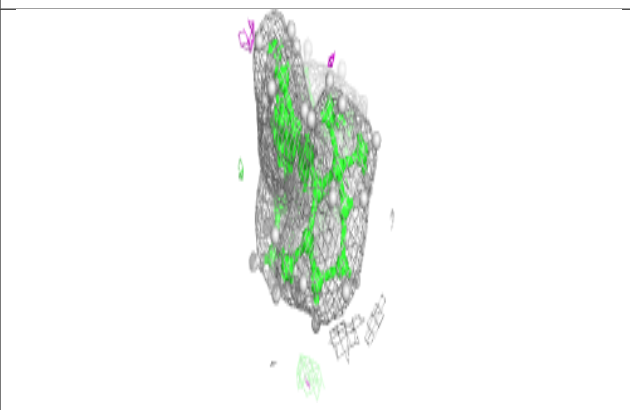
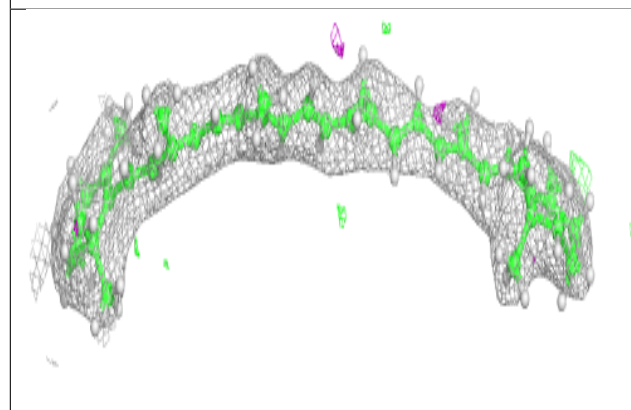
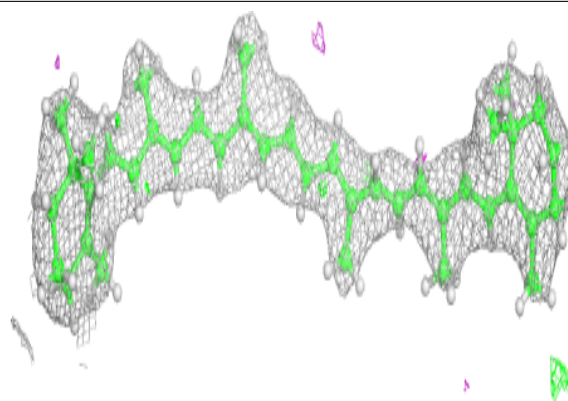
**Electron density around PHO a 406:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

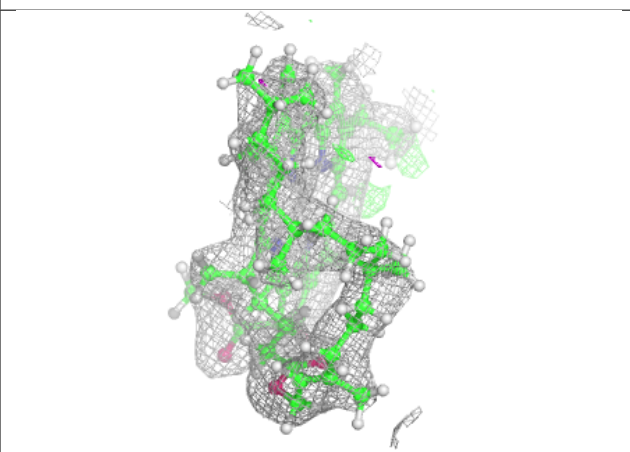
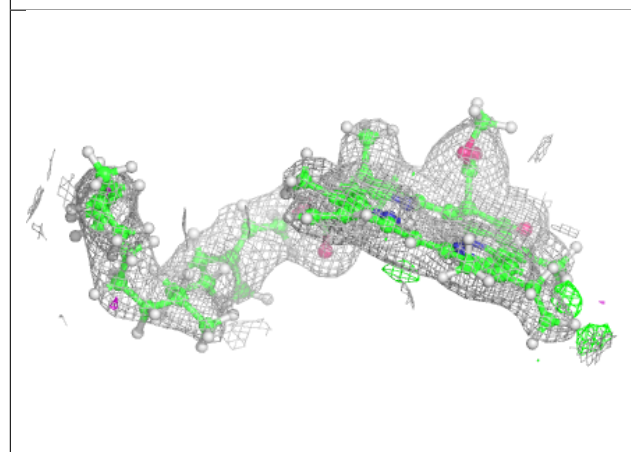
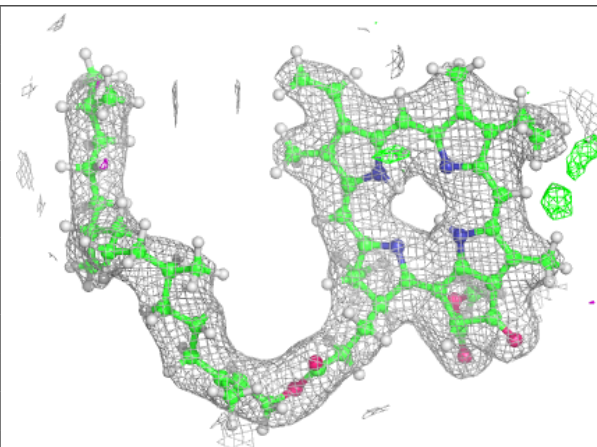


Electron density around BCR t 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

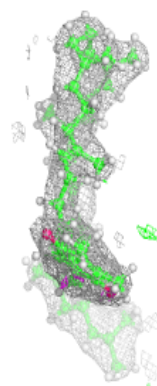
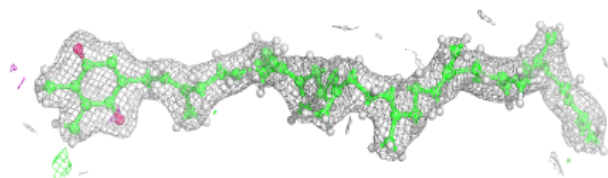
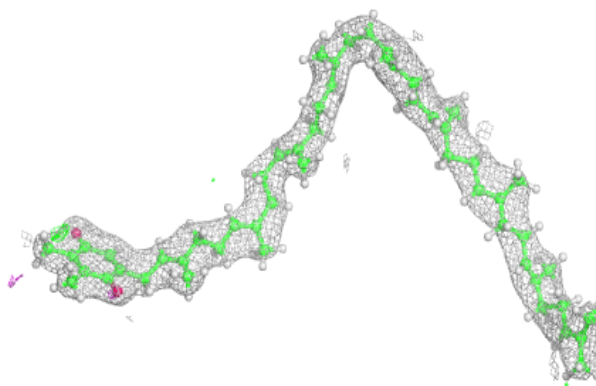
**Electron density around PHO d 402:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

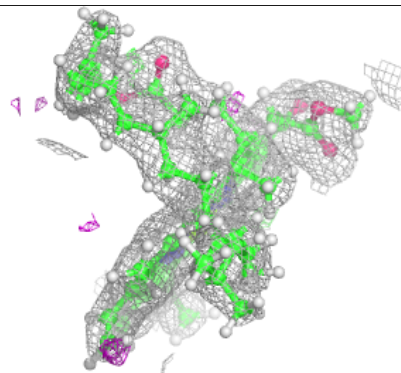
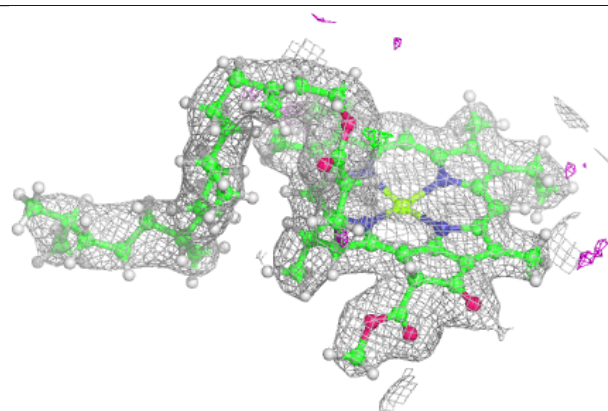
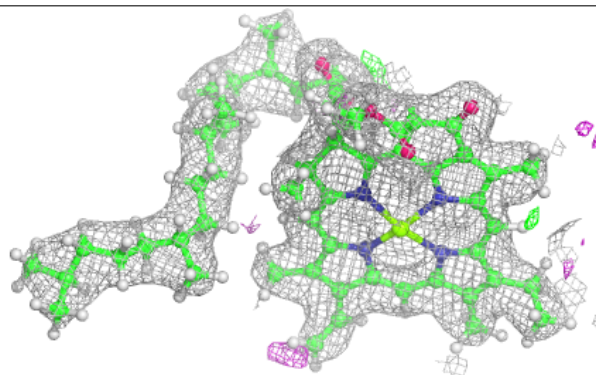


Electron density around PL9 D 406:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

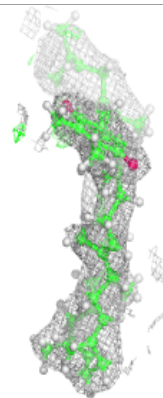
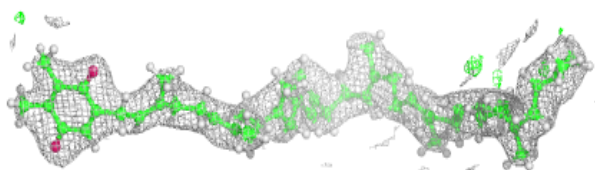
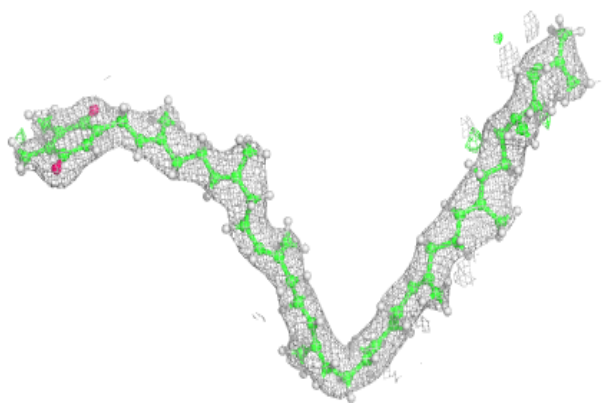
**Electron density around CLA D 402:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

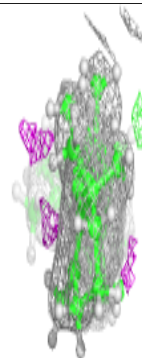
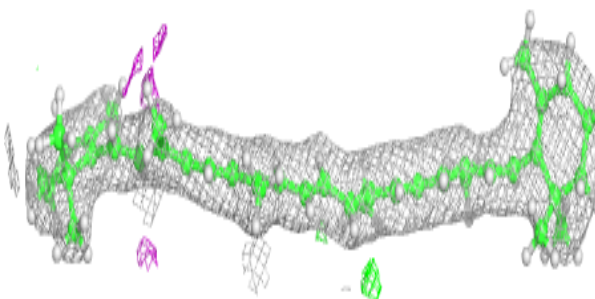
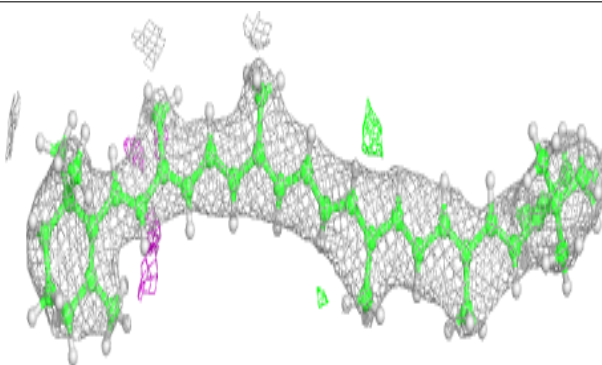


Electron density around PL9 d 407:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

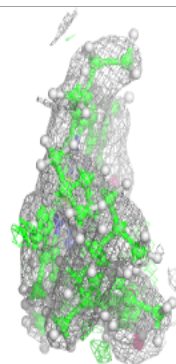
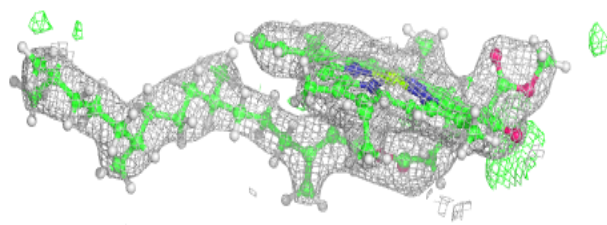
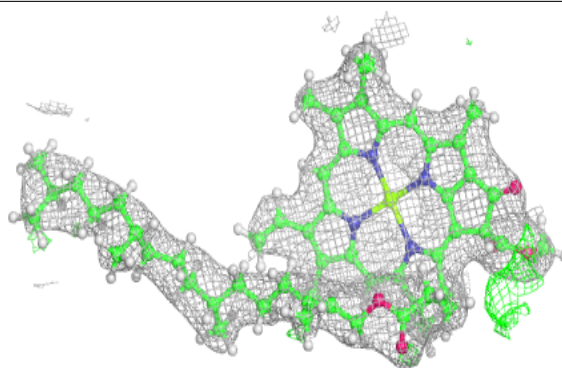
**Electron density around BCR B 617:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

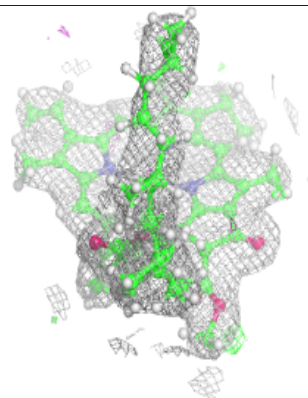
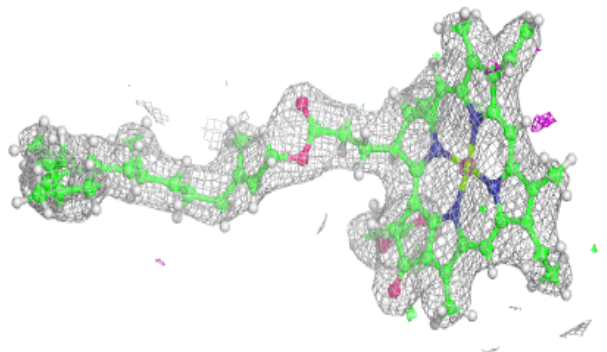
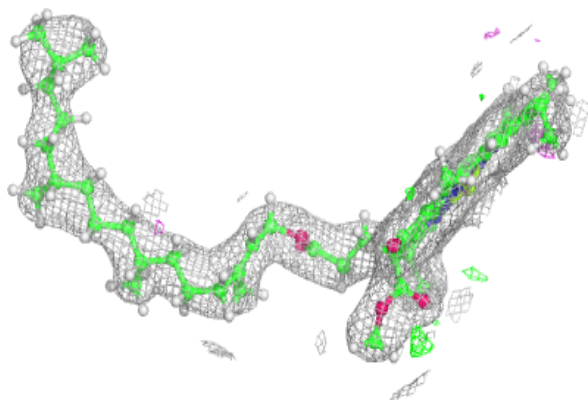


Electron density around CLA c 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

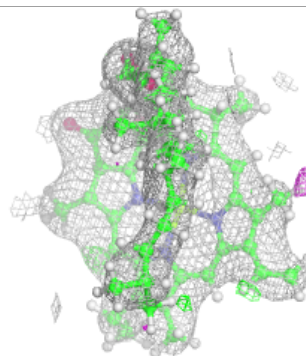
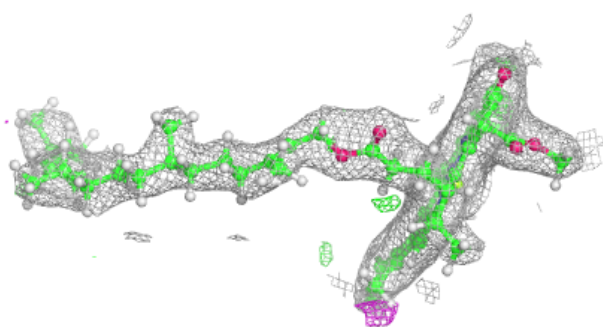
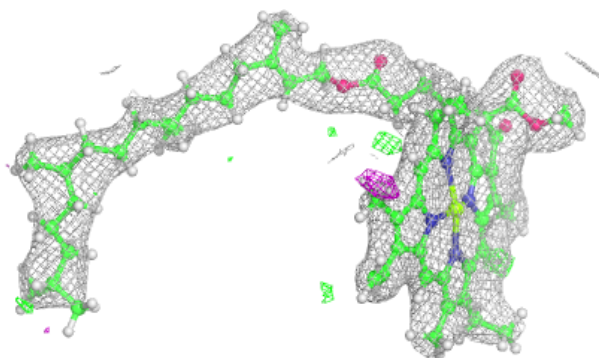
**Electron density around CLA D 403:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

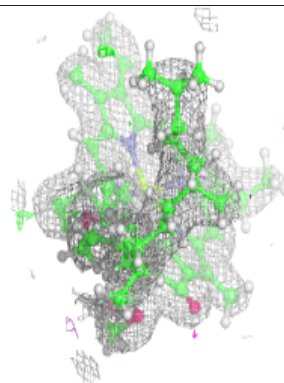
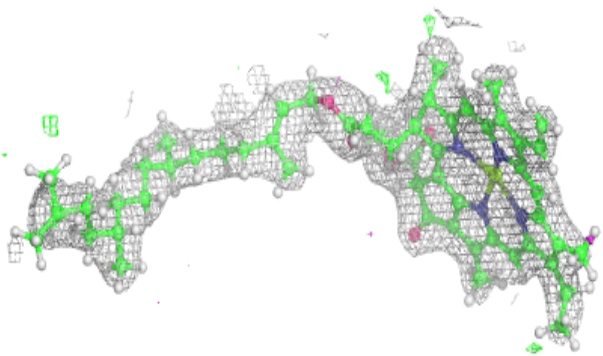
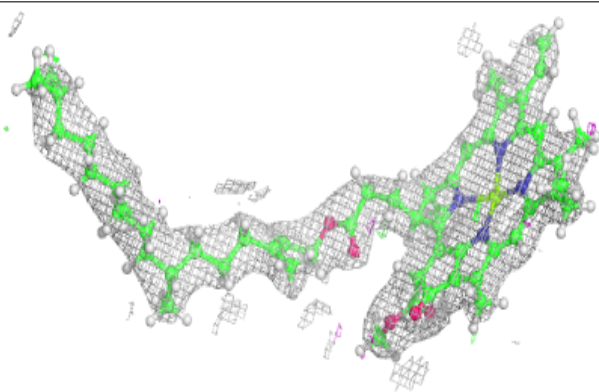


Electron density around CLA B 609:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

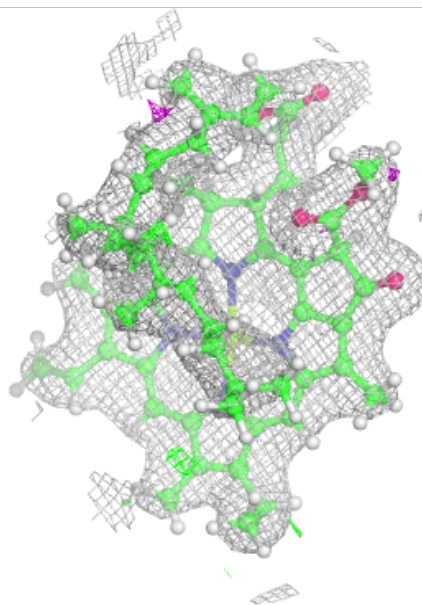
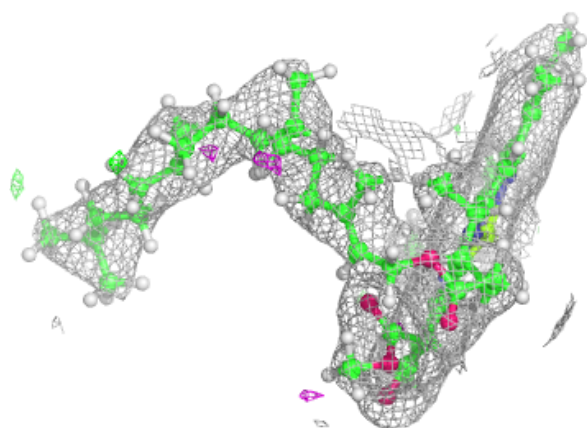
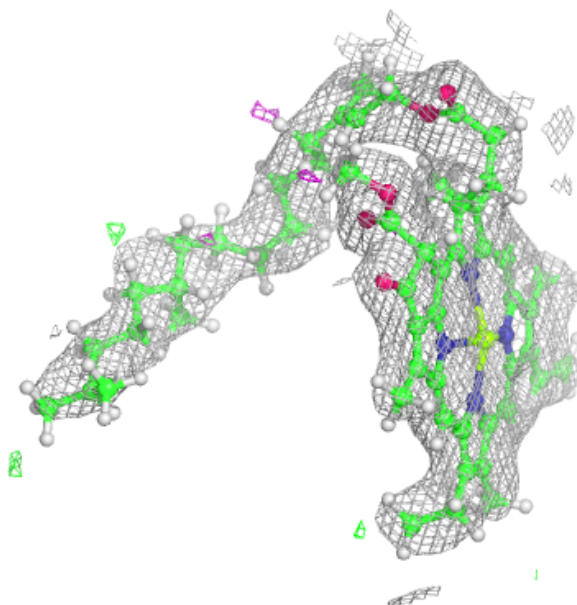
**Electron density around CLA a 404:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



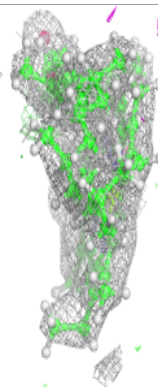
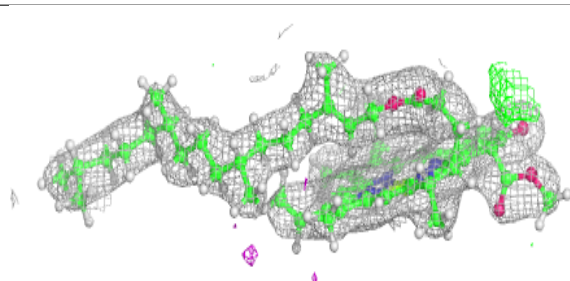
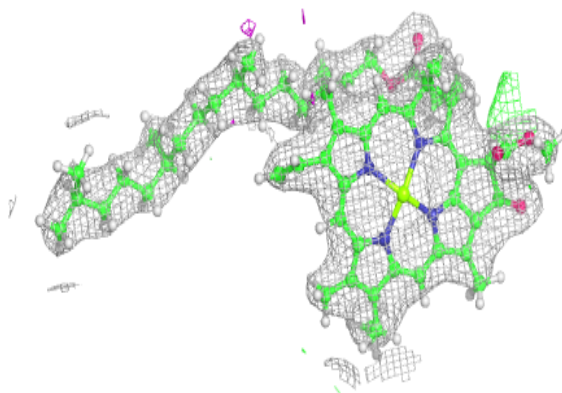
Electron density around CLA B 613:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

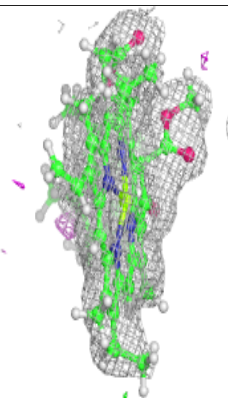
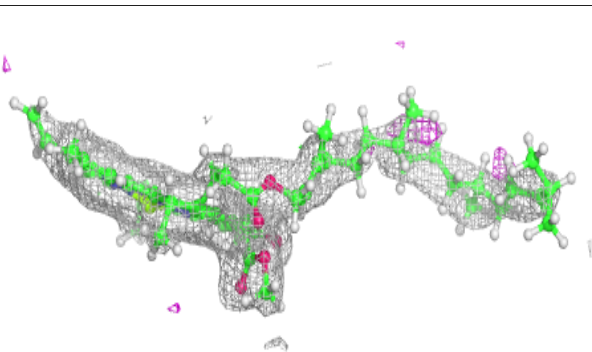
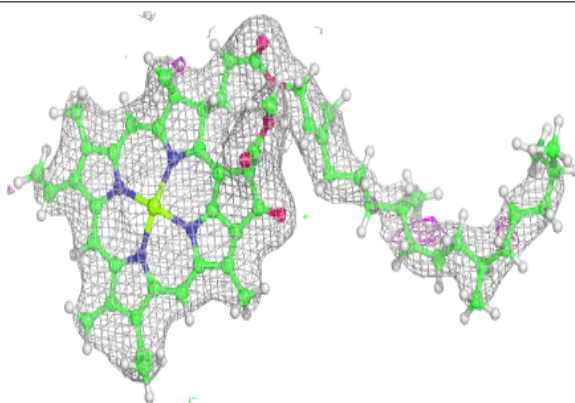


Electron density around CLA C 502:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

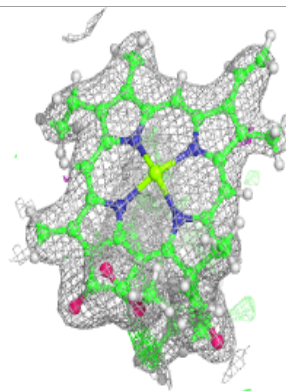
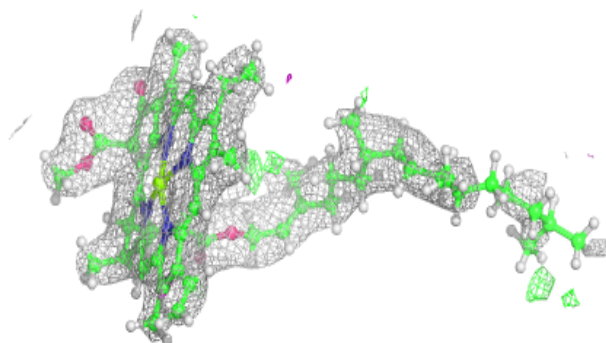
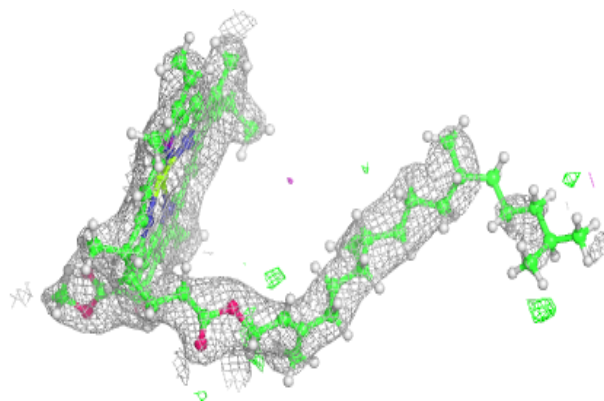
**Electron density around CLA b 603:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

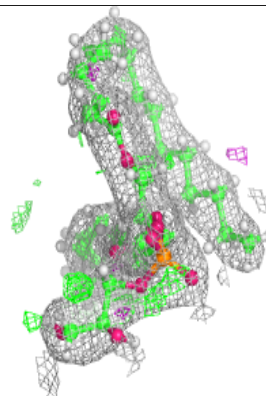
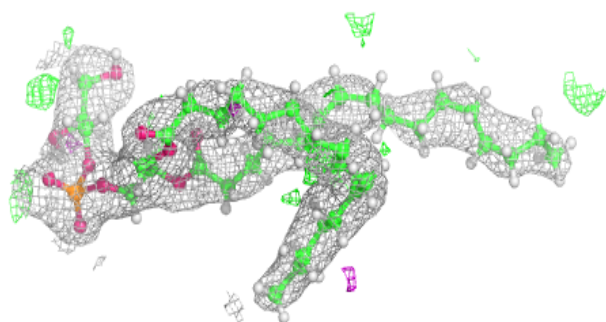
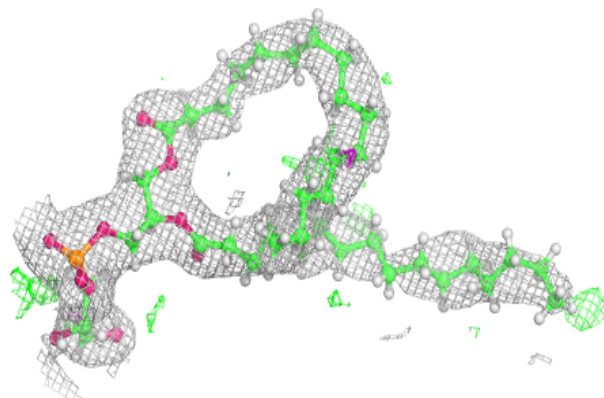


Electron density around CLA C 509:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

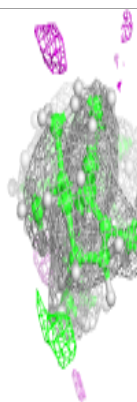
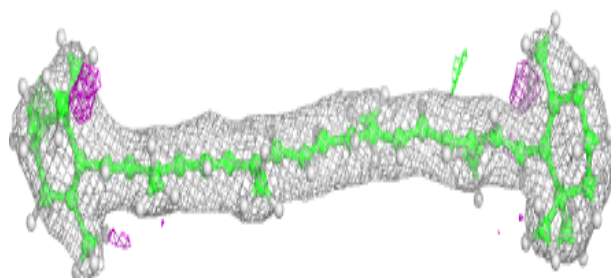
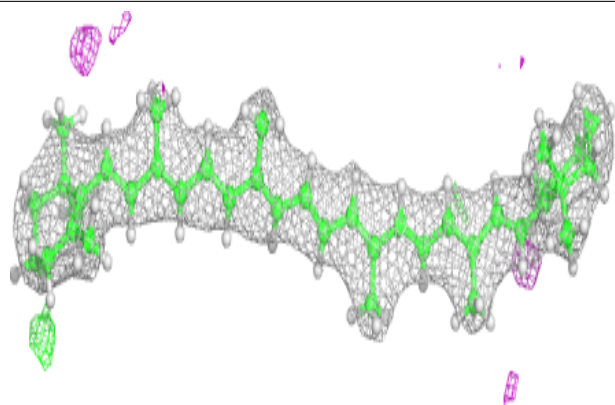
**Electron density around LHG D 411:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

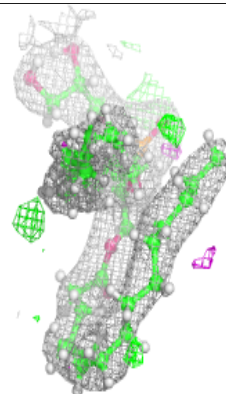
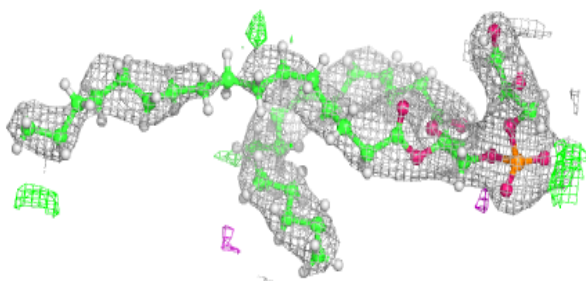
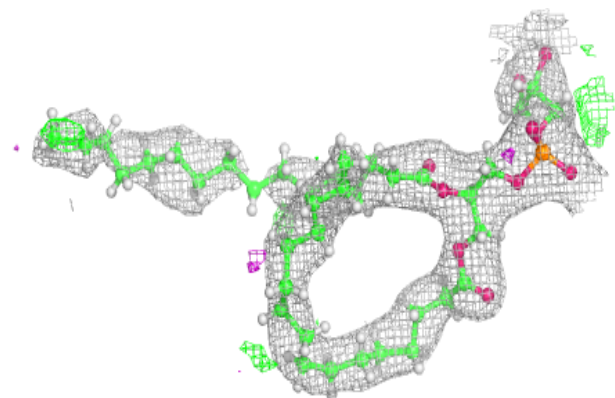


Electron density around BCR a 408:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

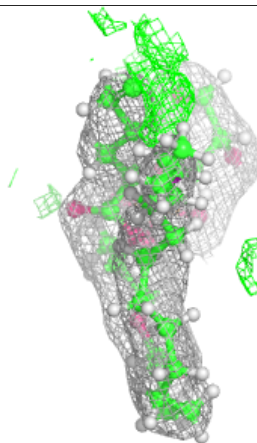
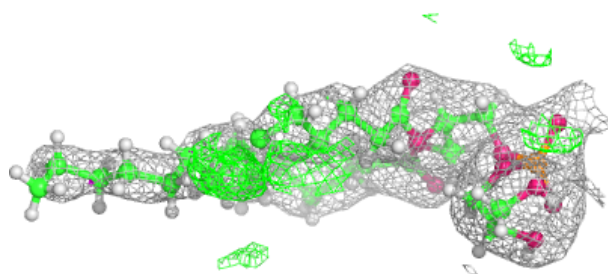
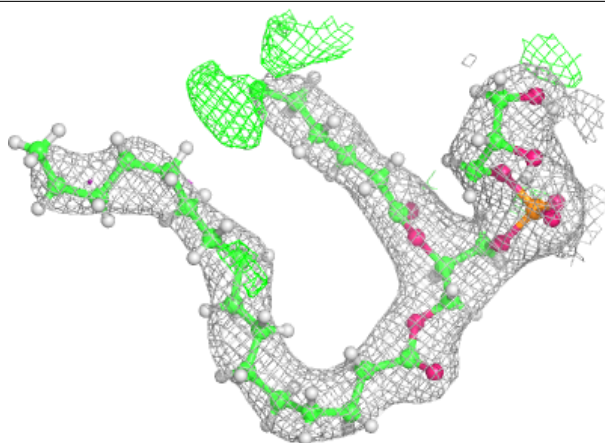
**Electron density around LHG d 408:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



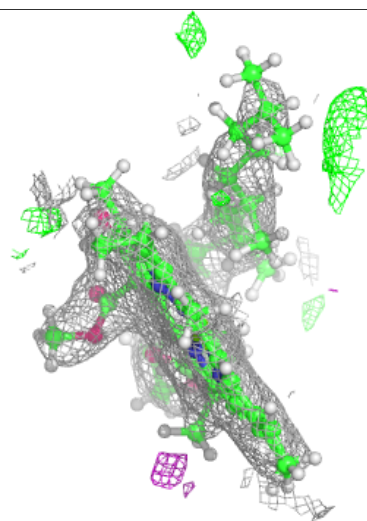
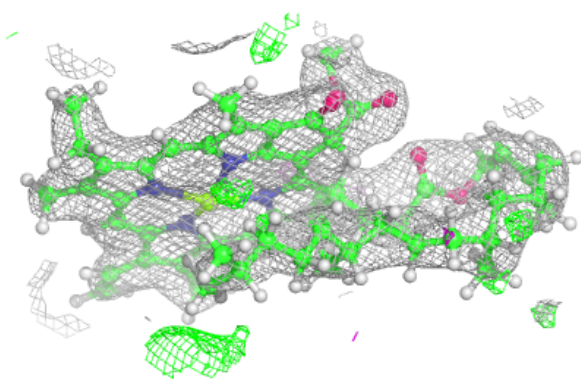
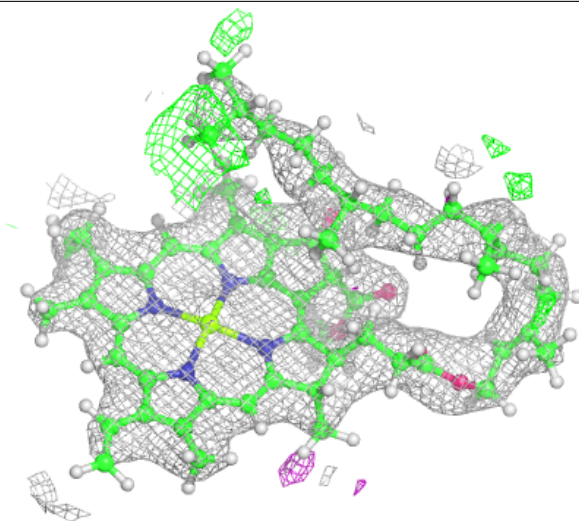
Electron density around LHG d 410:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



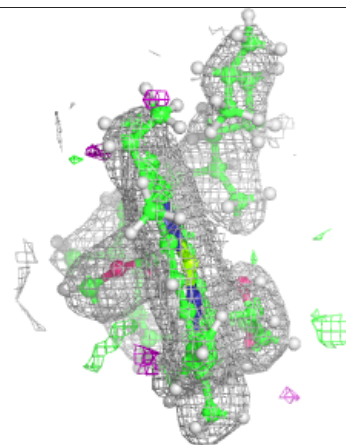
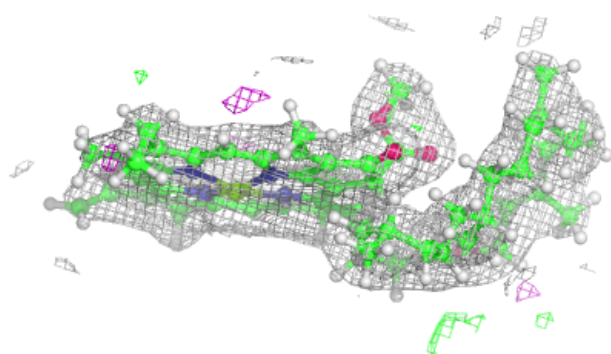
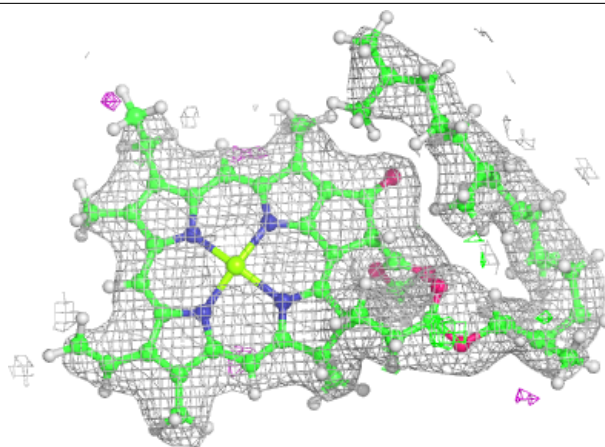
Electron density around CLA C 510:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

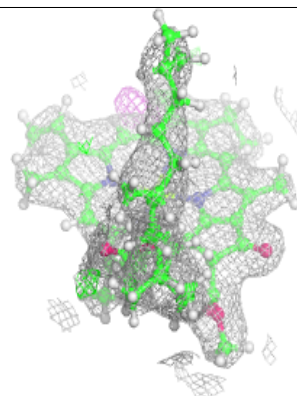
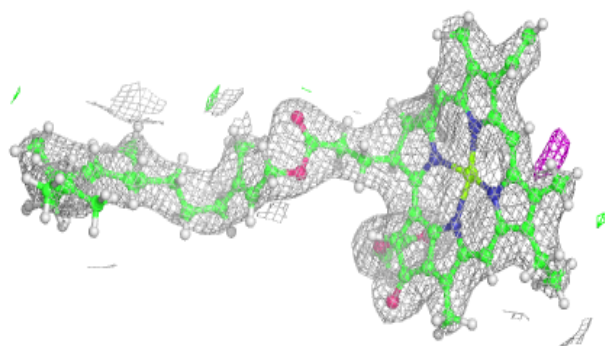
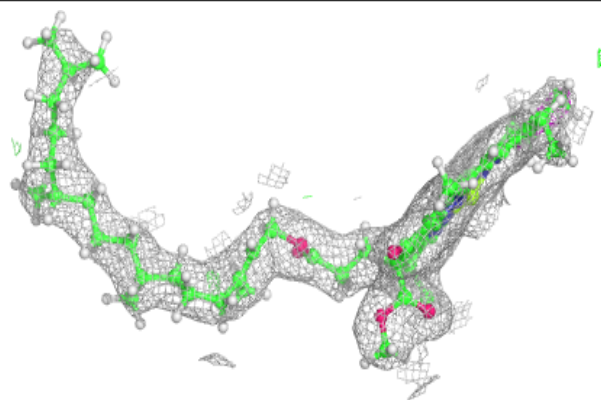


Electron density around CLA B 610:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

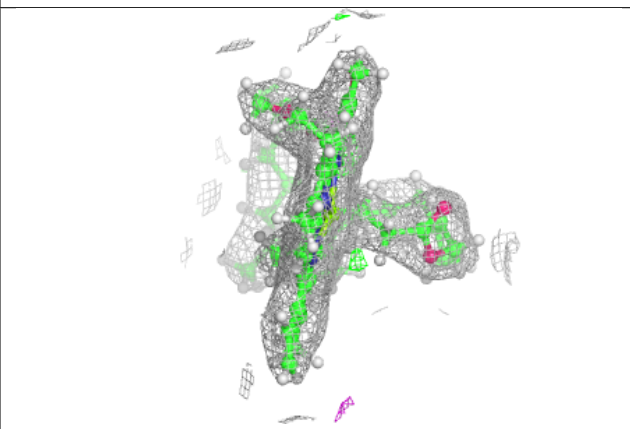
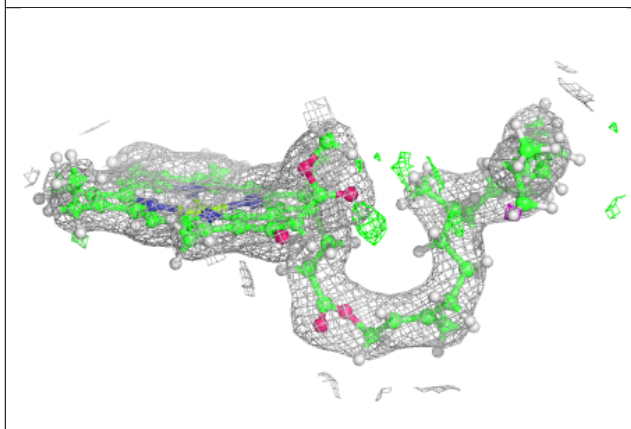
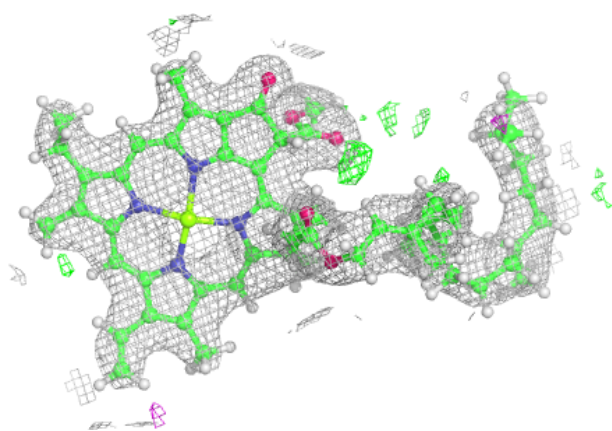
**Electron density around CLA d 404:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

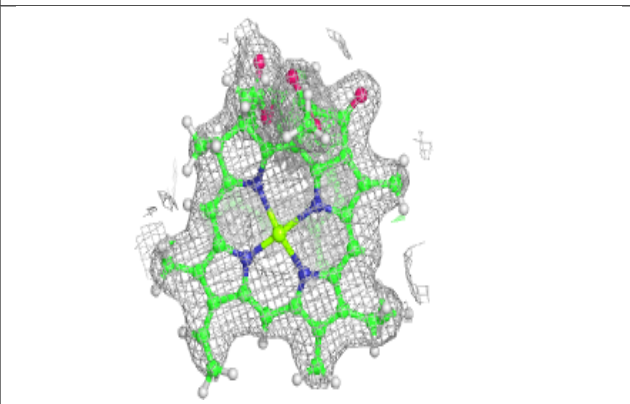
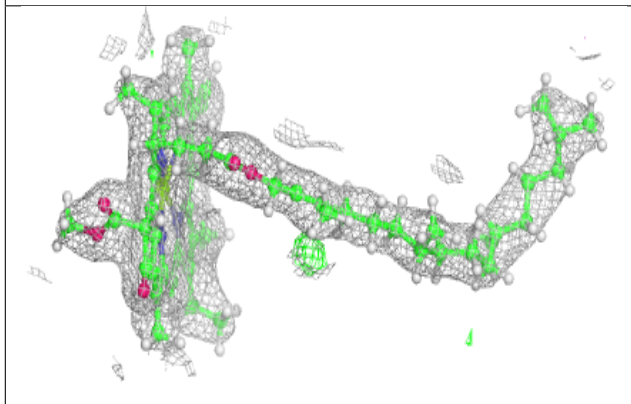
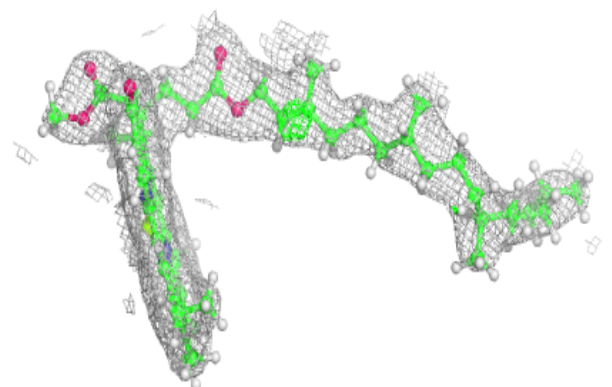


Electron density around CLA B 612:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

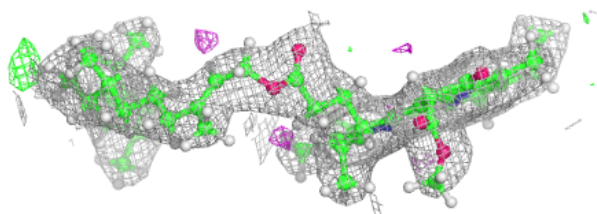
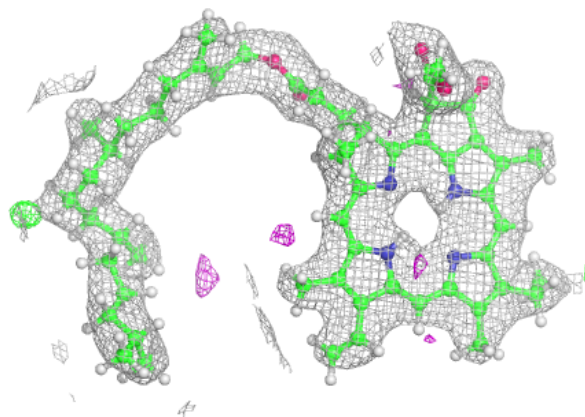
**Electron density around CLA b 606:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



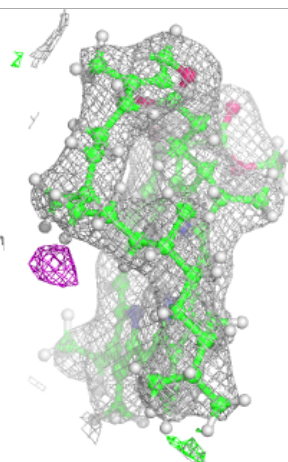
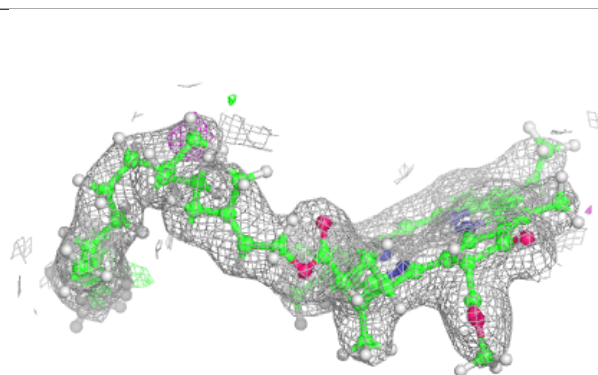
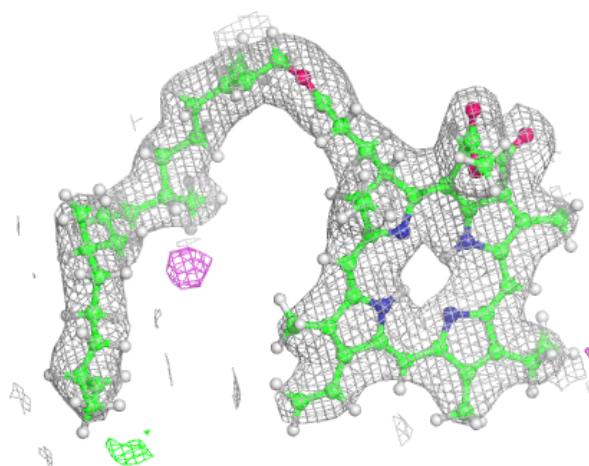
Electron density around PHO A 407:

$2mF_o-DF_c$ (at 0.7 rnsd) in gray
 mF_o-DF_c (at 3 rnsd) in purple (negative)
and green (positive)



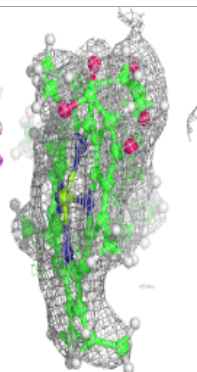
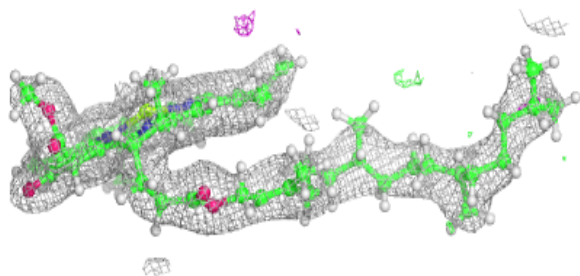
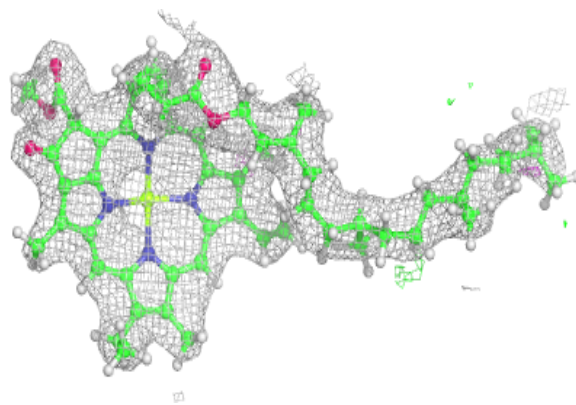
Electron density around PHO D 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

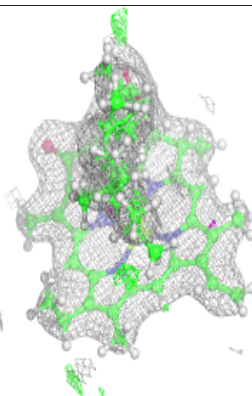
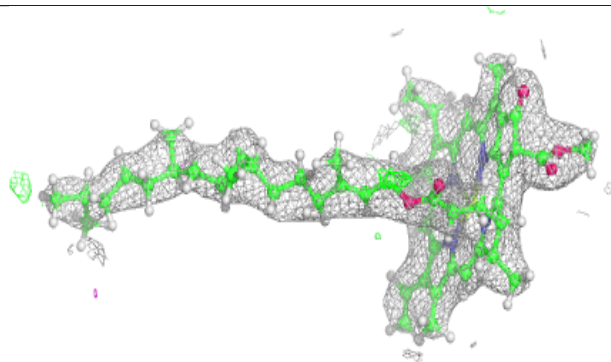
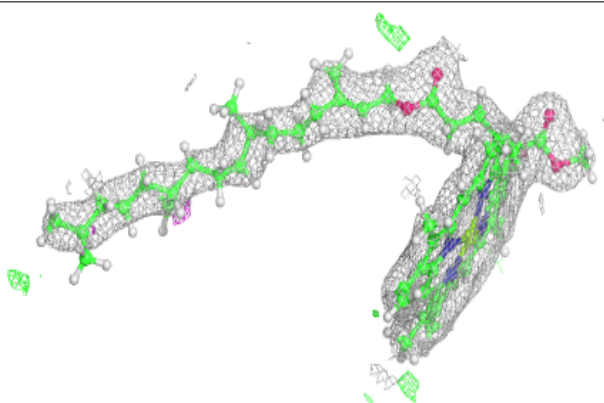


Electron density around CLA B 603:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

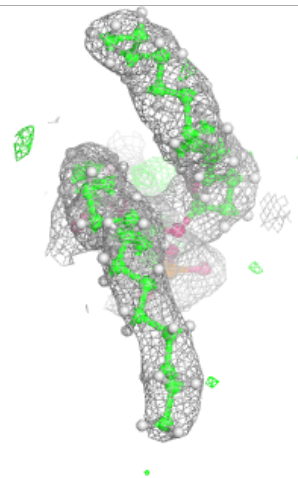
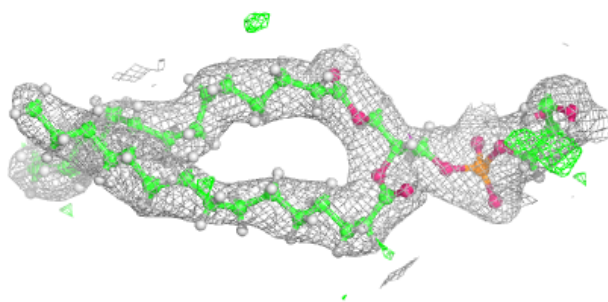
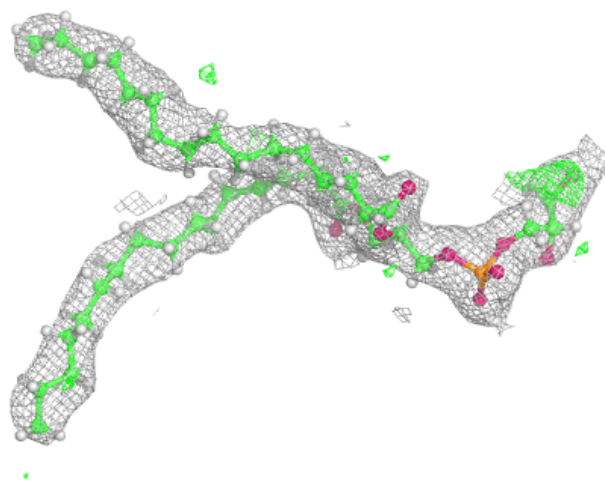
**Electron density around CLA b 608:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



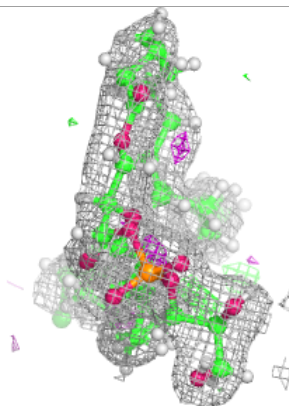
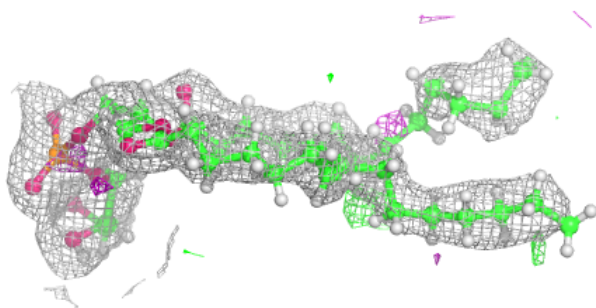
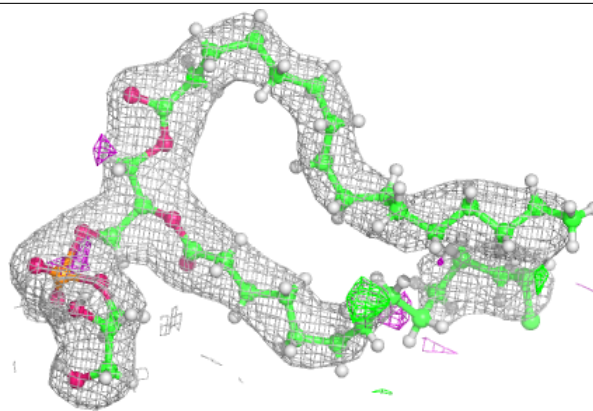
Electron density around LHG D 408:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

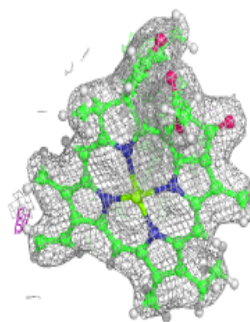
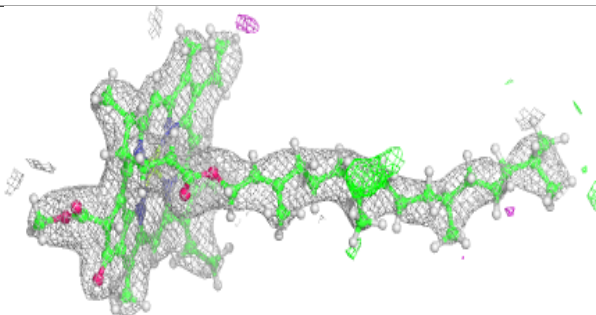
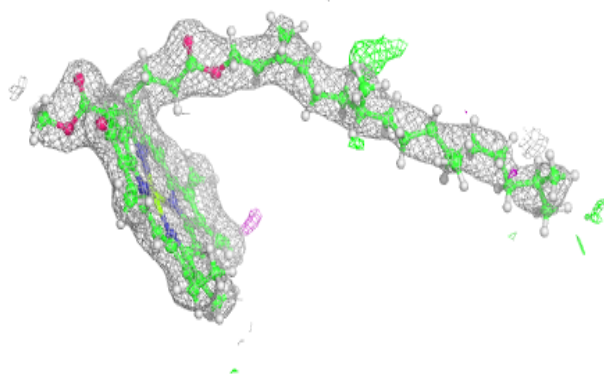


Electron density around LHG D 409:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

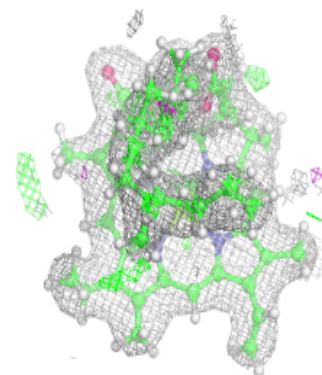
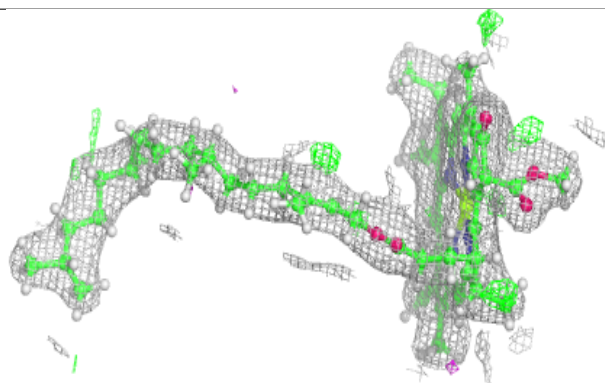
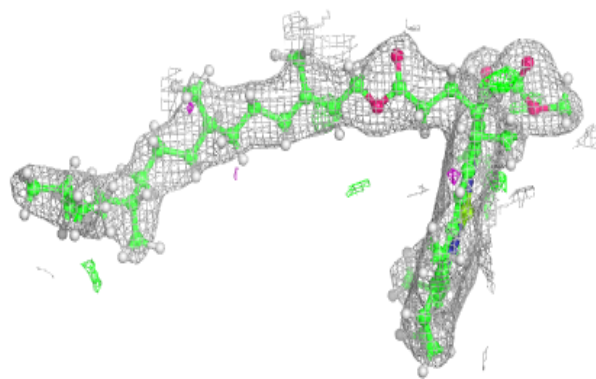
**Electron density around CLA B 607:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

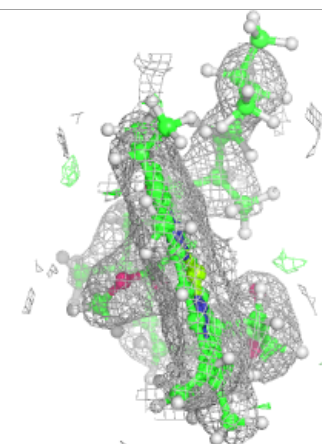
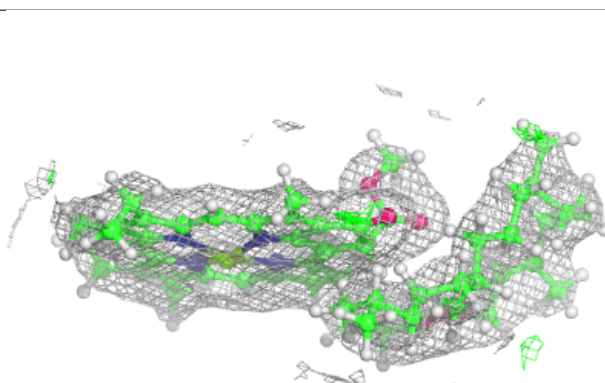
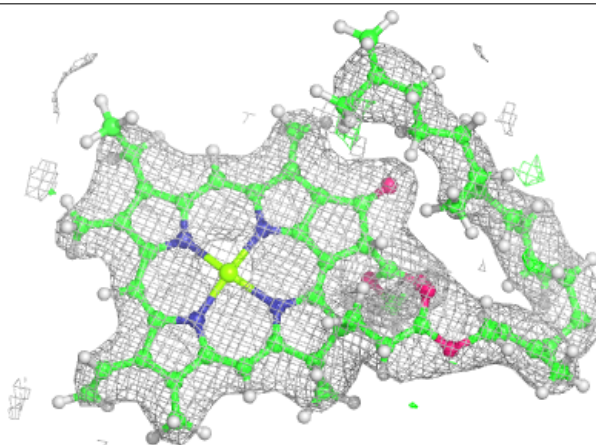


Electron density around CLA B 605:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

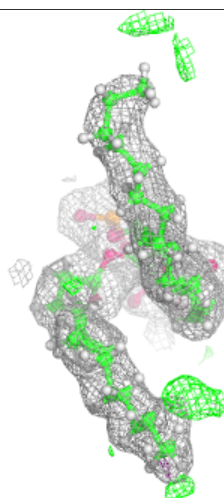
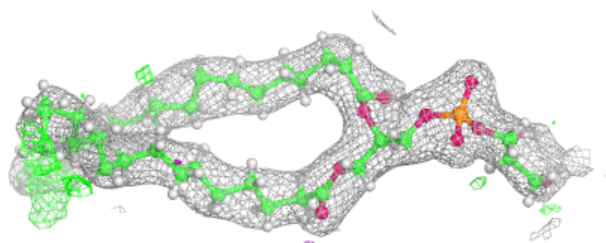
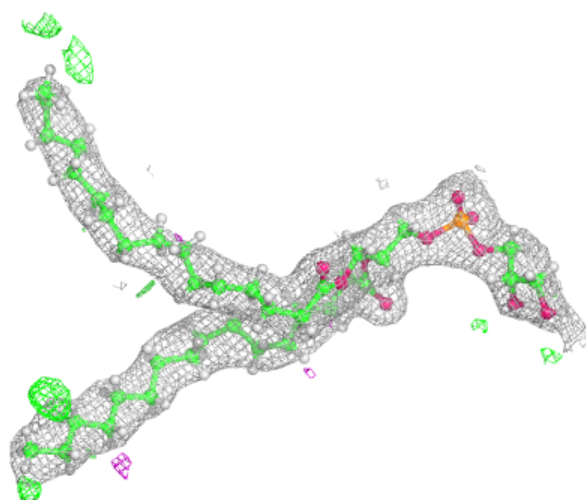
**Electron density around CLA b 611:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



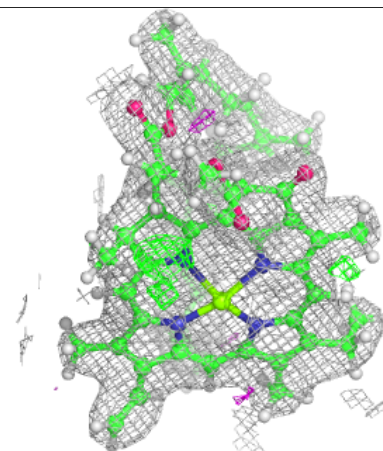
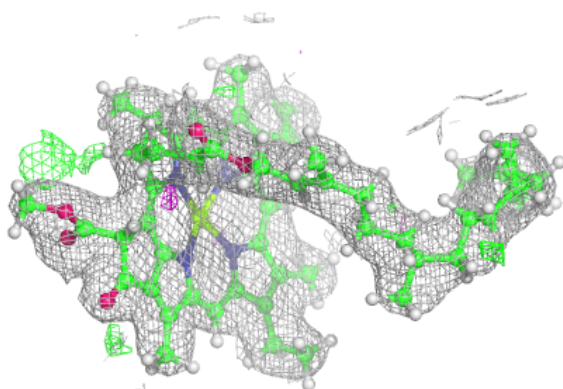
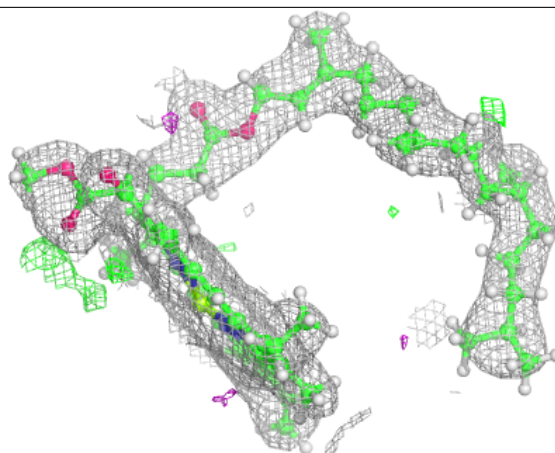
Electron density around LHG d 409:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

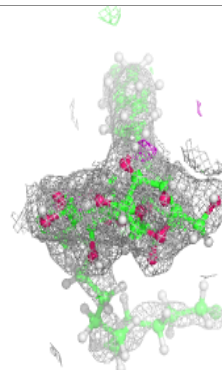
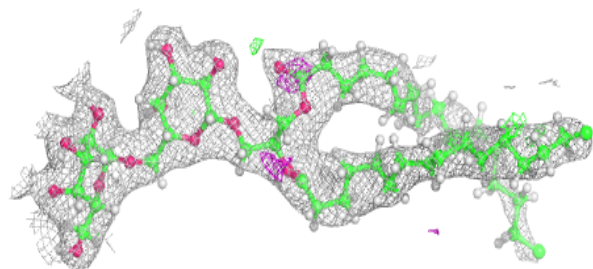
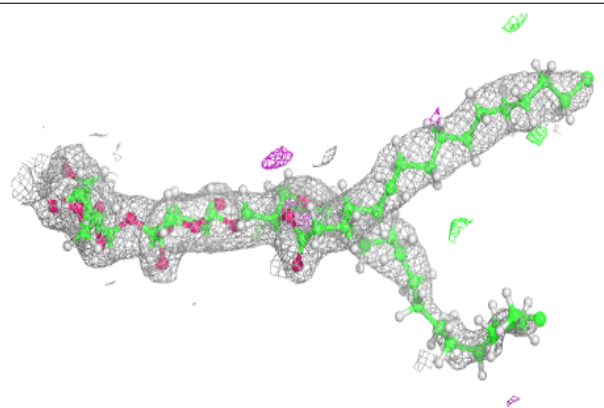


Electron density around CLA b 612:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

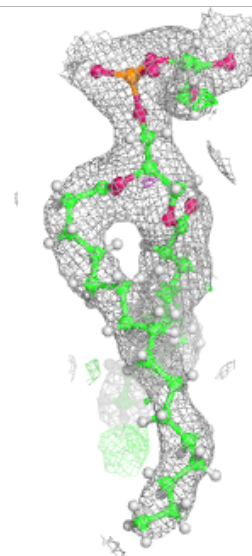
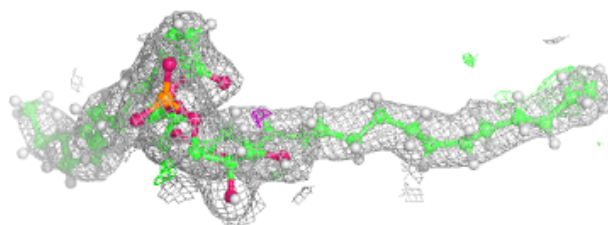
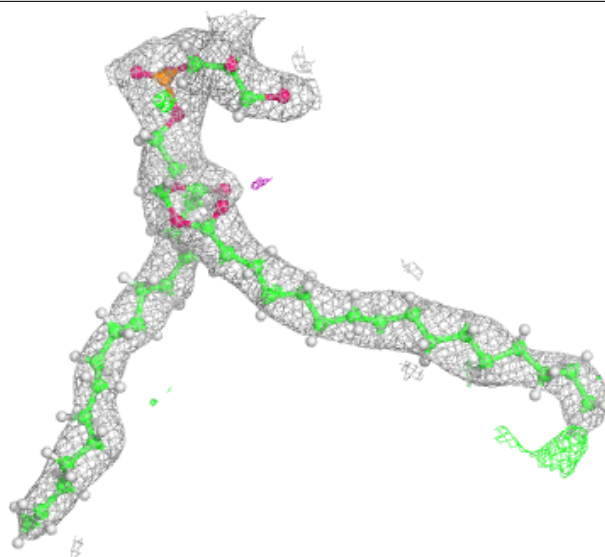
**Electron density around DGD c 516:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



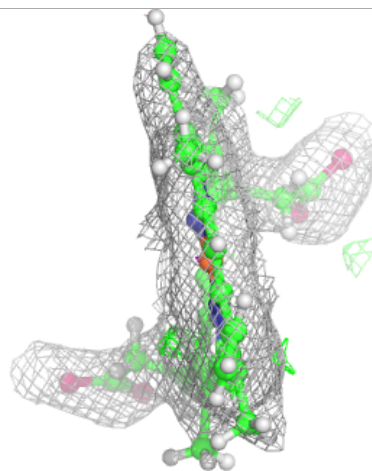
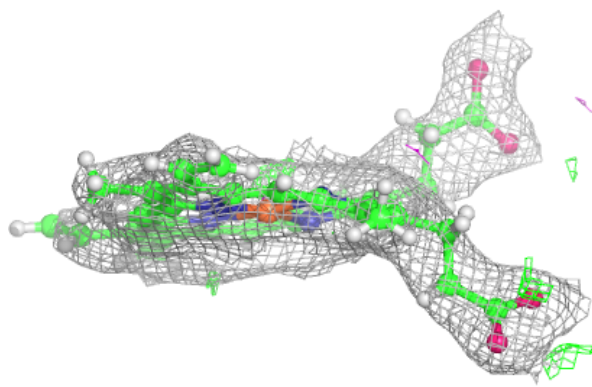
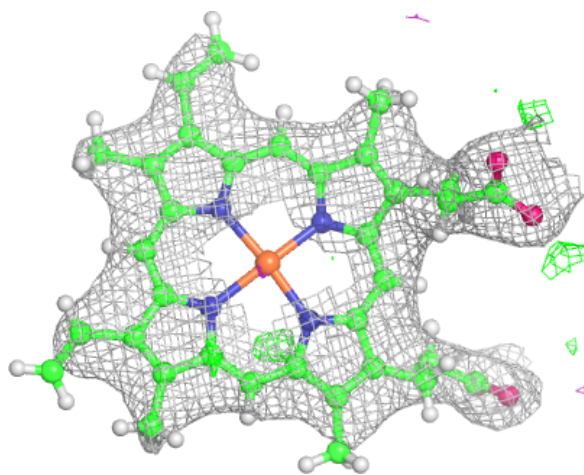
Electron density around LHG 1 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



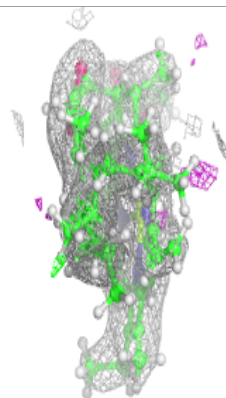
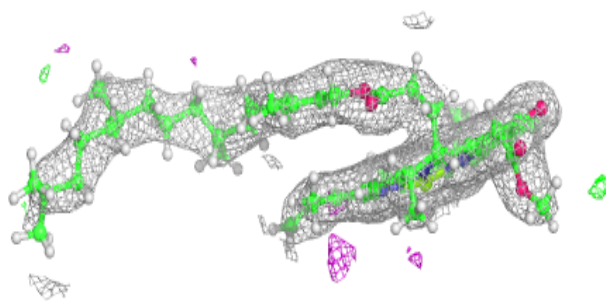
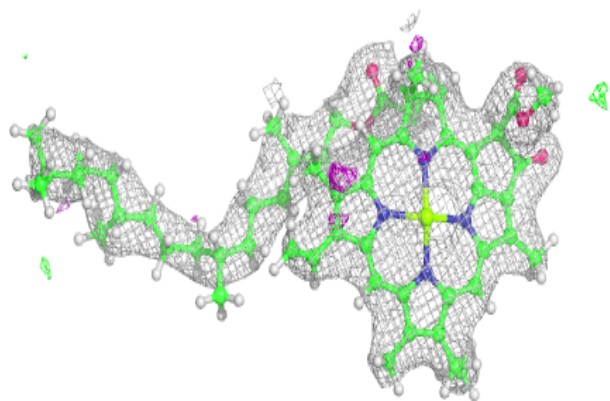
Electron density around HEM F 102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

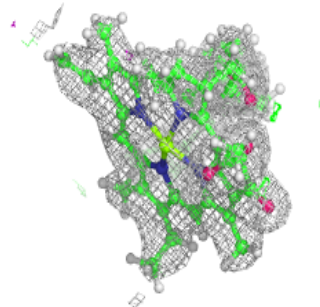
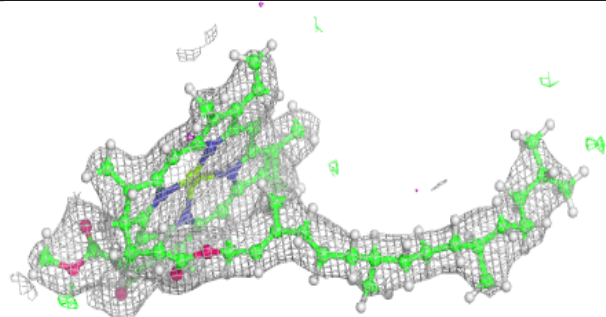
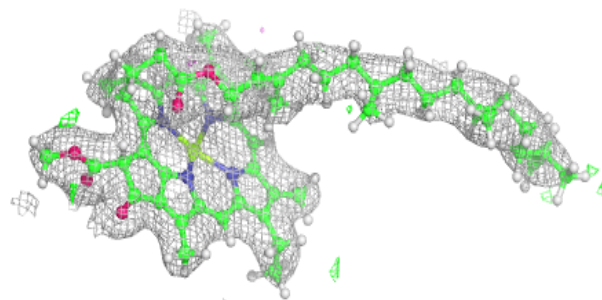


Electron density around CLA b 604:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

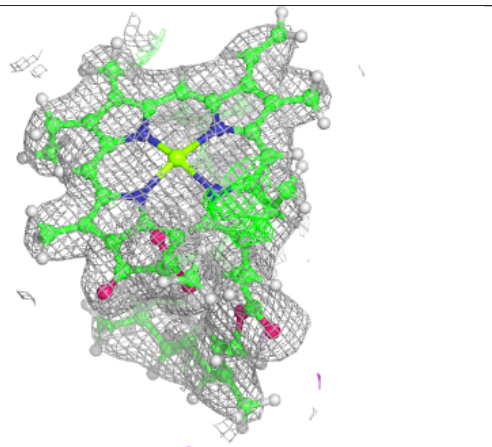
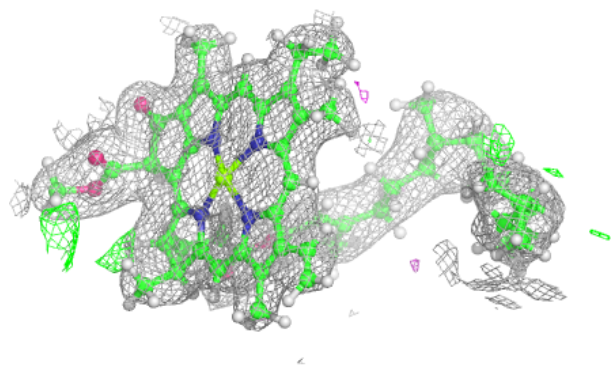
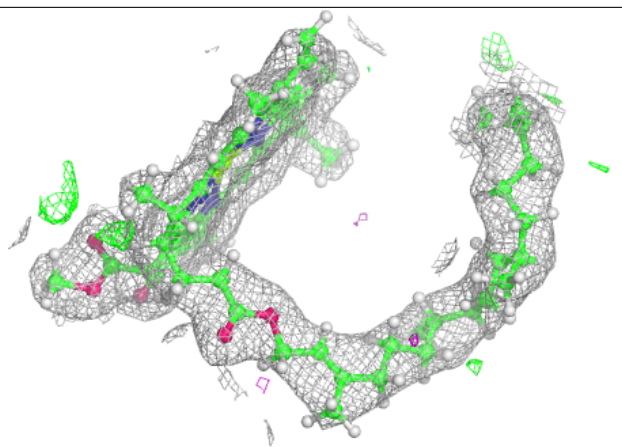
**Electron density around CLA B 608:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



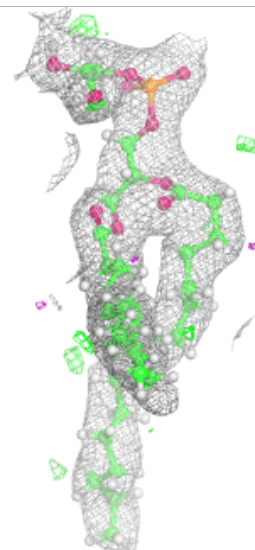
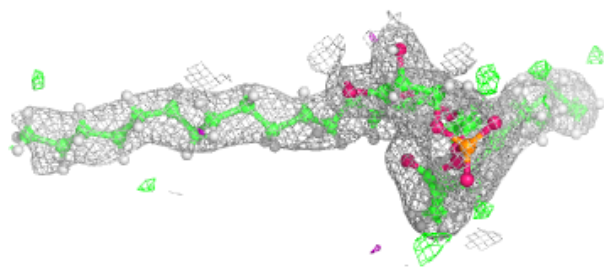
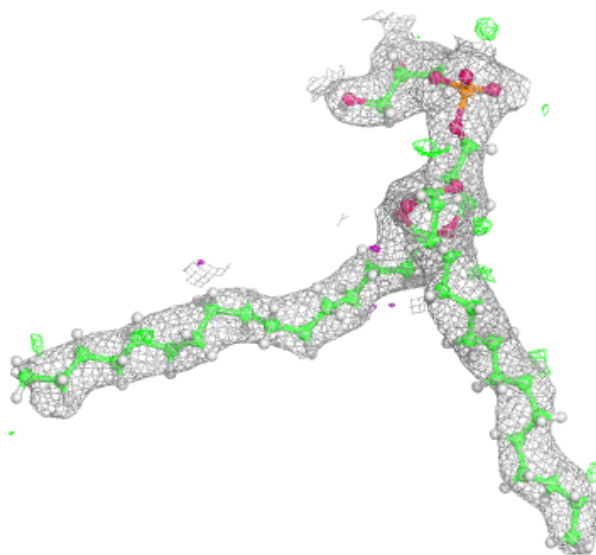
Electron density around CLA B 611:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



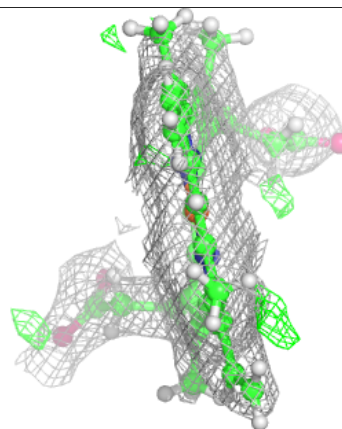
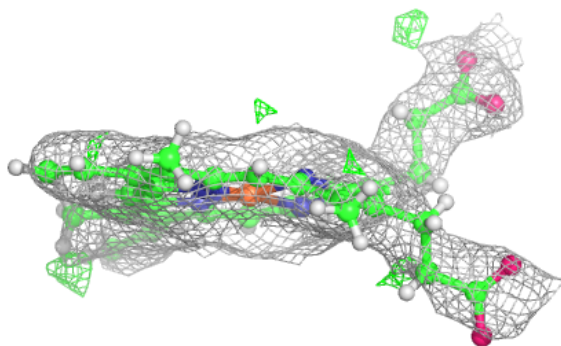
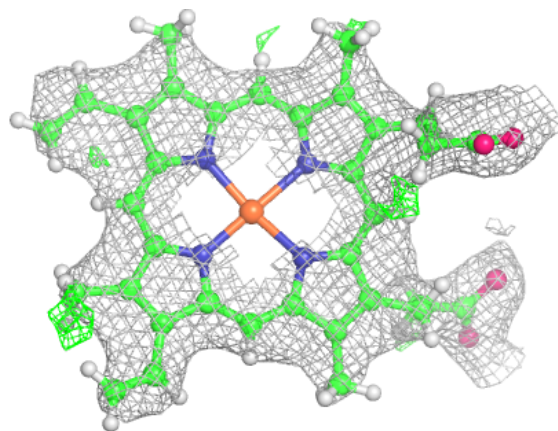
Electron density around LHG L 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



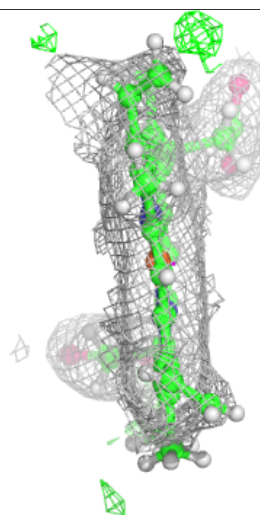
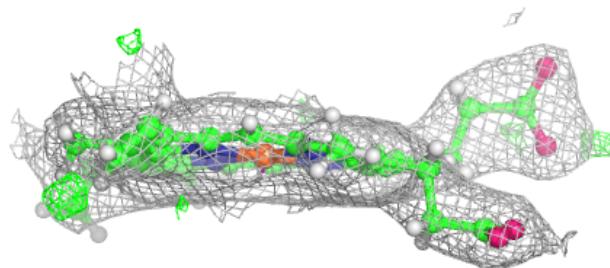
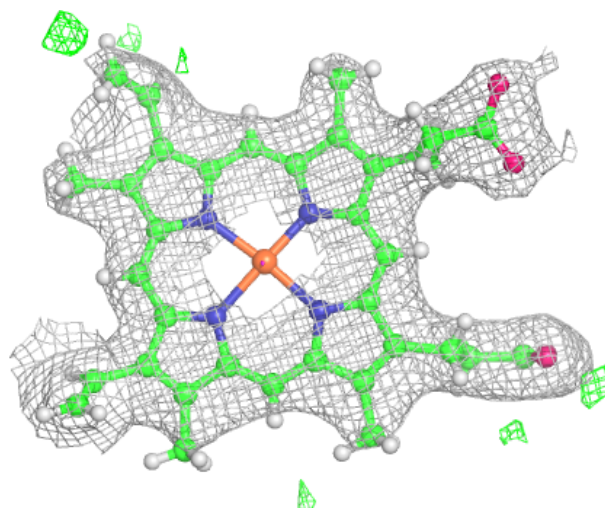
Electron density around HEM e 102:

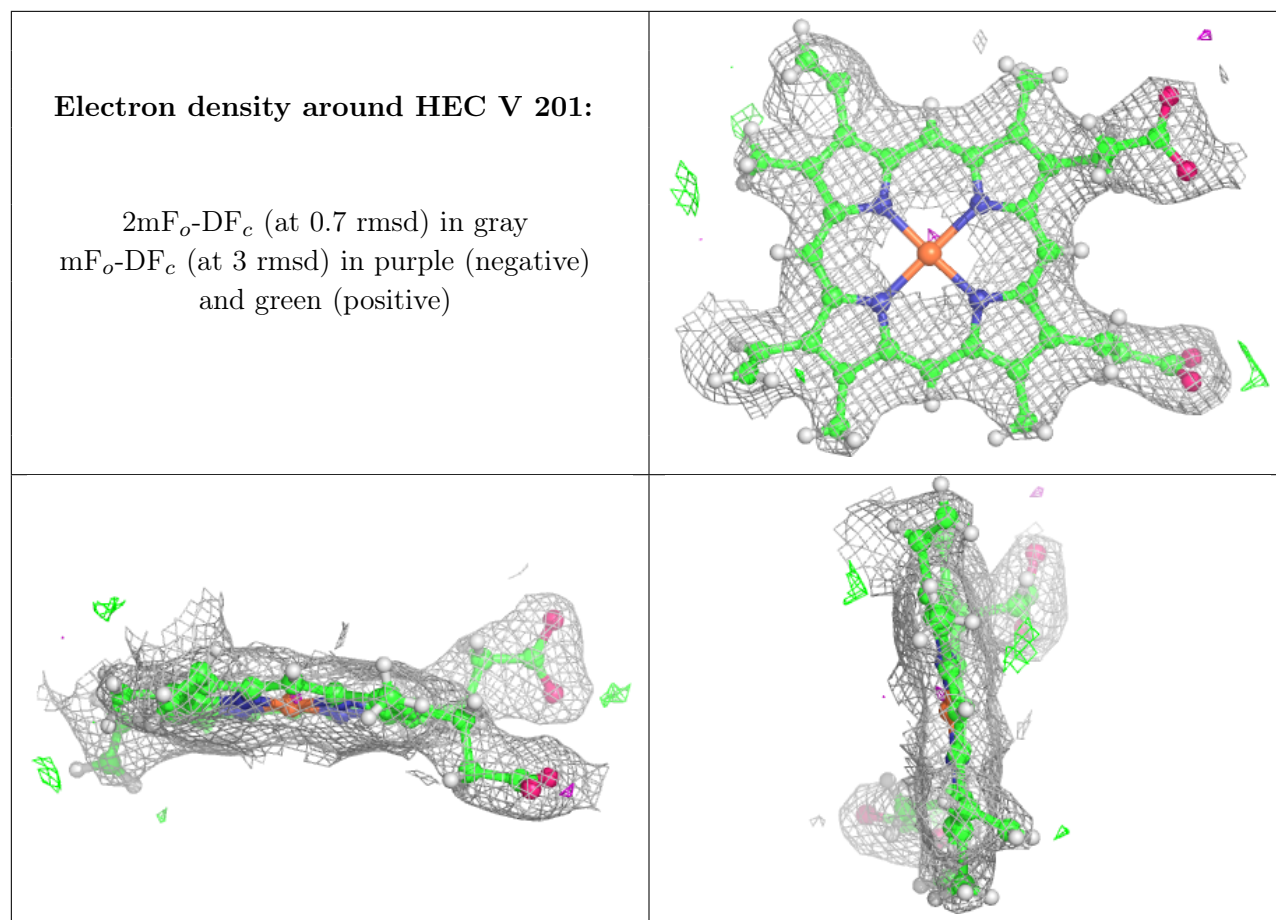
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEC v 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.